



Targeted Collaboration on Gas Turbine Combustion: Turbulent Lean Premixed Combustion with Hydrogen Enrichment

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Outline

Introduction & Motivation

Canadian Research Initiative

Mathematical Modelling

Computational Framework

Thickened Flame SFS Model

Flame Surface Density SFS Model

G-Equation SFS Model

Concluding Remarks



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- ▶ **Development of capabilities for modelling and prediction of premixed combustion under gas-turbine-like conditions**
 - ▶ high pressures and temperatures
 - ▶ lean hydrocarbon fuels with hydrogen enrichment
- ▶ **Lean Premixed Combustion with Hydrogen Enrichment**
 - ▶ high efficiency gas turbine combustion
 - ▶ reduced carbon dioxide production and NO_x emissions
 - ▶ paves the way for hydrogen combustion
- ▶ **Technical Challenges**
 - ▶ flame stability, sensitivity to fuel-to-air ratio fluctuations and thermo-acoustic oscillations
 - ▶ issues: local extinction, combustion instabilities, blow out, and flash back
 - ▶ **theoretical and computational models unable to fully explain experimental observations**

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Numerical Modelling of Premixed Combustion

Large Eddy Simulations (LES)

- ▶ intermediate between DNS and RANS: larger-scale motions resolved
- ▶ separation of scales via a low-pass spatial filtering procedure
- ▶ proving to be a valuable in modelling turbulent non-reacting flows
- ▶ while promising, still under development for turbulent reactive flows

Some of the Challenges

- ▶ complex chemical kinetics
- ▶ chemical reaction scales smaller than filter size
- ▶ in many cases, turbulence-chemistry interactions must be entirely modelled
- ▶ control of numerical, filtering (commutation and aliasing), subfilter scale modelling errors

Numerical Modelling of Premixed Combustion

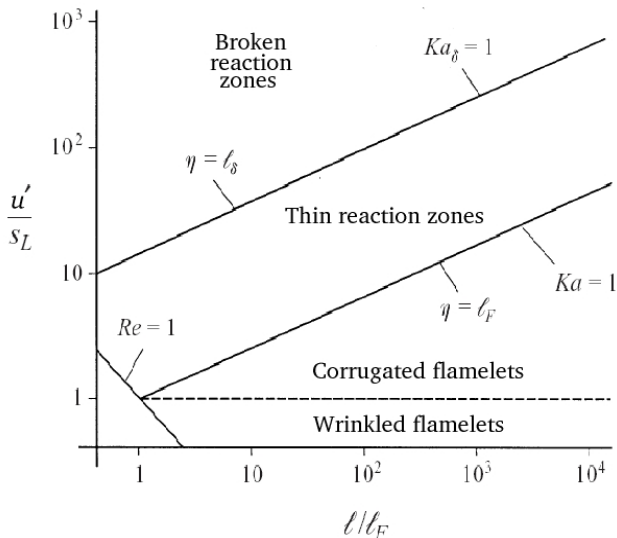
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Borghi-Peters Regime Diagram





Canadian Research Initiative

Collaborators

- ▶ Ö. Gülder and C. Groth (University of Toronto)
- ▶ G. Smallwood, F. Liu, H. Guo (NRC ICPET)
- ▶ 7-8 graduate students

Research

- ▶ Numerical and experimental research program
- ▶ 5 numerical tasks
- ▶ 3 experimental tasks

A Key Outcome

- ▶ development of Large Eddy Simulation (LES) capabilities for turbulent lean premixed combustion



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Numerical Tasks

- ▶ **Subgrid Scale Modelling**: Thickened Flame with Power-Law Flame Wrinkling Subgrid Scale Model for Lean-Premixed Combustion
- ▶ **Subgrid Scale Modelling**: Flame Surface Density (FSD) Subgrid Scale Model for Lean-Premixed Combustion
- ▶ **Subgrid Scale Modelling**: G-Equation Subgrid Scale Model for Lean-Premixed Combustion
- ▶ **LES**: Development of Grid-Independent LES Capabilities for Turbulent Reacting Flows
- ▶ **Hydrogen Enrichment**: Effects of Hydrogen/Reformation Gas Addition on Flammability Limit and NO_x Emission in Lean Counterflow CH₄/Air Premixed Flames

LES Filtering

Low-pass spatial filtering of flow quantities \mathcal{G} :

$$\bar{\mathcal{G}}(\mathbf{x}, t) = \int \int \int_{V_{sf}} F(\mathbf{x} - \mathbf{x}'; \Delta(\mathbf{x})) \mathcal{G}(\mathbf{x}', t) d^3 \mathbf{x}'$$

Mass-weighted (Favre) spatial filtering:

$$\bar{\rho} \tilde{\mathcal{G}}(\mathbf{x}, t) = \int \int \int_{V_{sf}} \rho F(\mathbf{x} - \mathbf{x}'; \Delta(\mathbf{x})) \mathcal{G}(\mathbf{x}', t) d^3 \mathbf{x}'$$

Consistency:

$$\int \int \int_{V_{sf}} F(\mathbf{x} - \mathbf{x}') d^3 \mathbf{x}' = 1$$

Filtered Navier-Stokes Equations

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_j)}{\partial x_j} = 0$$

$$\frac{\partial (\bar{\rho} \tilde{u}_i)}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_i \tilde{u}_j + \delta_{ij} \bar{p})}{\partial x_j} - \frac{\partial \tilde{\sigma}_{ij}}{\partial x_j} = - \underbrace{\frac{\partial \tau_{ij}}{\partial x_j}}_{\text{I}} + \underbrace{\frac{\partial (\bar{\sigma}_{ij} - \tilde{\sigma}_{ij})}{\partial x_j}}_{\text{II}}$$

$$\frac{\partial (\bar{\rho} \tilde{Y}_n)}{\partial t} + \frac{\partial (\bar{\rho} \tilde{Y}_n \tilde{u}_j)}{\partial x_j} + \frac{\partial \tilde{J}_{j,n}}{\partial x_j} = - \underbrace{\frac{\partial [\bar{\rho} (\widetilde{Y_n u_j} - \tilde{Y}_n \tilde{u}_j)]}{\partial x_j}}_{\text{IX}} - \underbrace{\frac{\partial (\bar{J}_{j,n} - \tilde{J}_{j,n})}{\partial x_j}}_{\text{X}} + \underbrace{\tilde{\dot{\omega}}_n}_{\text{XI}}$$

$$\bar{p} = \bar{\rho} R \tilde{T} + \underbrace{\sum_{n=1}^N R_n \bar{\rho} (\widetilde{Y_n T} - \tilde{Y}_n \tilde{T})}_{\text{XII}}$$

Filtered Navier-Stokes Equations

$$\begin{aligned}
 \frac{\partial(\bar{\rho}\tilde{E})}{\partial t} + \frac{\partial[(\bar{\rho}\tilde{E} + \bar{p})\tilde{u}_j]}{\partial x_j} - \frac{\partial(\tilde{\sigma}_{ij}\tilde{u}_i)}{\partial x_j} + \frac{\partial\tilde{q}_j}{\partial x_j} = & \underbrace{- \frac{\partial[\bar{\rho}(\widetilde{u_j h_s} - \tilde{u}_j \tilde{h}_s)]}{\partial x_j}}_{\text{III}} \\
 & + \underbrace{\frac{\partial(\bar{\sigma}_{ij}\tilde{u}_i - \tilde{\sigma}_{ij}\tilde{u}_i)}{\partial x_j}}_{\text{IV}} + \underbrace{\frac{\partial(\overline{u_i \sigma_{ij}} - \tilde{u}_i \tilde{\sigma}_{ij})}{\partial x_j}}_{\text{V}} \\
 & - \underbrace{\frac{1}{2} \frac{\partial[\bar{\rho}(\widetilde{u_j u_i u_i} - \bar{\rho} \tilde{u}_j \tilde{u}_i \tilde{u}_i)]}{\partial x_j}}_{\text{VI}} + \underbrace{\frac{\partial(\bar{q}_j - \tilde{q}_j)}{\partial x_j}}_{\text{VII}} \\
 & - \underbrace{\frac{\partial[\sum_{n=1}^N \Delta h_{f,n}^0 \bar{\rho}(\widetilde{Y_n u_j} - \tilde{Y}_n \tilde{u}_j)]}{\partial x_j}}_{\text{VIII}}
 \end{aligned}$$

Subfilter Scale Modelling and Closures

- ▶ Subfilter scale stresses (term **I**): $\tau_{ij} = -2\mu_t \left(\tilde{S}_{ij} - \frac{1}{3} \delta_{ij} \tilde{S}_{ll} \right) + \frac{2}{3} \delta_{ij} \tilde{\rho} \tilde{k}$
 - ▶ eddy-viscosity models
 - ▶ Smagorinsky (1963) & Yoshizawa (1986) models
 - ▶ one-equation model

- ▶ Subfilter scale scalar transport (term **IX**):

$$\tilde{\rho}(\widetilde{Y_n u_j} - \tilde{Y}_n \tilde{u}_j) = -\frac{\mu_t}{Sc_t} \frac{\partial \tilde{Y}_n}{\partial x_j}$$

- ▶ Subfilter scale enthalpy transport (term **III**):

$$\tilde{\rho}(\widetilde{u_j h_s} - \tilde{u}_j \tilde{h}_s) = -\frac{\mu_t}{Pr_t} \frac{\partial \tilde{T}}{\partial x_j}$$

- ▶ Subfilter turbulent diffusion (term **VI**, Knight *et al.* , 1998):

$$\frac{\tilde{\rho}(\widetilde{u_j u_i u_i} - \tilde{\rho} \tilde{u}_j \tilde{u}_i \tilde{u}_i)}{2} = \tau_{ij} \tilde{u}_i$$

Subfilter Scale Stress Models

Smagorinsky & Yoshizawa Models

Smagorinsky eddy-viscosity model (1963):

$$\tau_{ij} - \frac{\delta_{ij}}{3}\tau_{kk} = -2\bar{\rho}\nu_t\tilde{S}_{ij}, \quad \nu_t = C_s^2\Delta^2|\tilde{S}|, \quad |\tilde{S}| = (2\tilde{S}_{ij}\tilde{S}_{ij})^{1/2}, \quad C_s \approx 0.10-0.24$$

Yoshizawa model (1986):

$$\tau_{kk} = C_I 2\bar{\rho}\Delta^2|\tilde{S}|^2, \quad C_I \approx 0.09-0.005$$

One-Equation Model

Eddy-viscosity:

$$\nu_t = C_v\sqrt{k}\Delta, \quad C_v \approx 0.086-0.09$$

\tilde{k} -equation:

$$\frac{\partial(\bar{\rho}\tilde{k})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{k}\tilde{u}_i)}{\partial x_i} = P - \epsilon + \frac{\partial}{\partial x_k} \left(\bar{\rho} \frac{\nu_t}{Pr_t} \frac{\partial \tilde{k}}{\partial x_k} \right)$$

Turbulence-Chemistry Interaction Models

Modelling Approaches for Premixed Combustion

- ▶ **Thickened Flame Model**
 - ▶ Butler & O'Rourke, 1977; Colin *et al.* , 2000
 - ▶ power-law flame wrinkling model (Charlette *et al.* , 2002)
- ▶ **Flame-Surface Density (FSD) Model**
 - ▶ Hawkes & Cant, 2000, 2001; Tullis & Cant, 2003
- ▶ **G-Equation Model**
 - ▶ Williams, 1985; Kerstein & Williams, 1988; Peters, 2000; Pitsch & Duchamp de Lageneste, 2002
- ▶ **Laminar Flamelet Models**
 - ▶ models based on the flamelet concept
 - ▶ Bray *et al.* , 1985; Peters, 1999;

Computational Framework

Key Elements I:

- ▶ **Finite-Volume Formulation**
 - ▶ reliable, robust, & accurate spatial discretizations
- ▶ **Block-Based Adaptive Mesh Refinement**
 - ▶ body-fitted multi-block mesh
 - ▶ local anisotropic mesh refinement
- ▶ **Parallel Implementation Via Domain Decomposition**
 - ▶ efficient and scalable algorithm
- ▶ **Low-Mach Number Local Preconditioning**
 - ▶ Weiss & Smith (1995)

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Computational Framework

Key Elements II:

- ▶ **Parallel Implicit Time-Marching Scheme**
 - ▶ Newton-Krylov-Schwarz (NKS) approach for steady combustion (Keys and co-researchers, 1998, 2001; Groth & Northrup, 2005)
 - ▶ dual-time-stepping approach for unsteady combustion
- ▶ **Development for Laminar and RANS**
 - ▶ Northrup & Groth, 2005; Gao & Groth, 2005

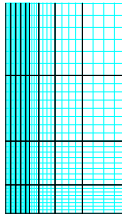


Computational Framework

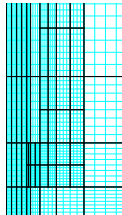
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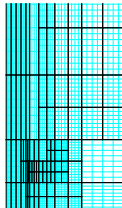
Non-Premixed Laminar Diffusion Flame



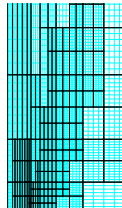
Initial Level
96 Blocks (4x8)
3072 Cells



2 Levels of Refinement
126 Blocks (4x8)
4032 Cells

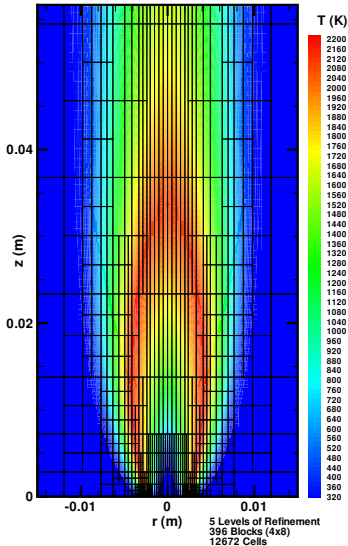


3 Levels of Refinement
195 Blocks (4x8)
6240 Cells

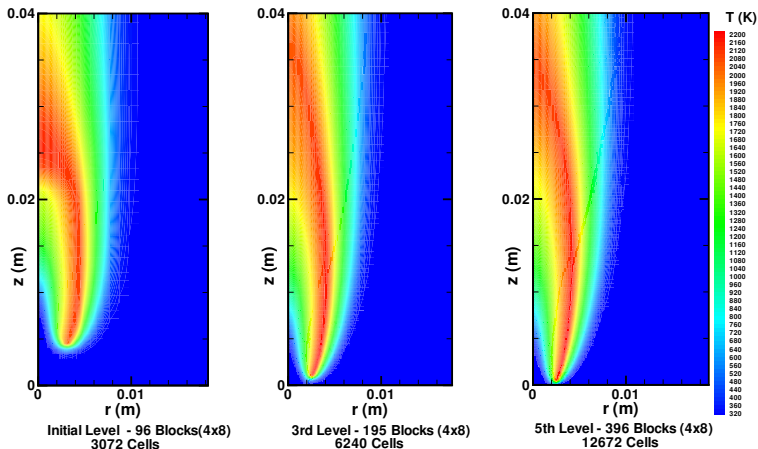


4 Levels of Refinement
327 Blocks (4x8)
10464 Cells

Groth and Gülder

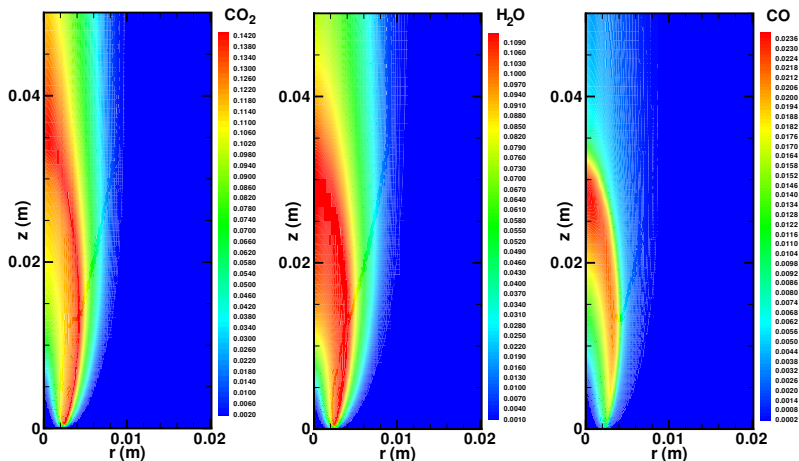


Non-Premixed Laminar Diffusion Flame



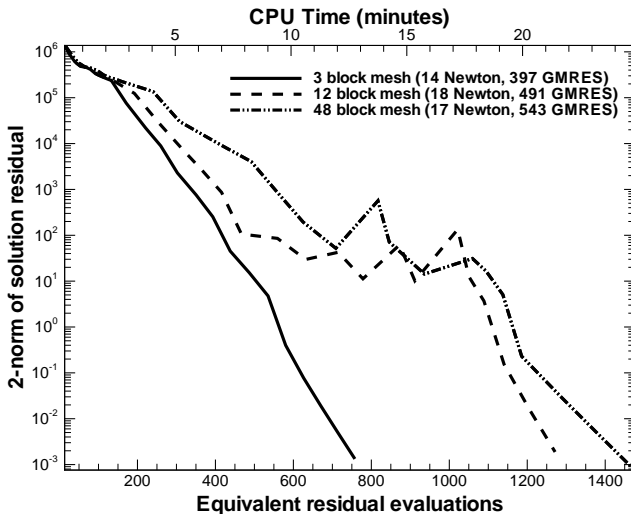
5 refinements, 5 levels of refinement, 396 (4x8) blocks = 12672 cells

Non-Premixed Laminar Diffusion Flame



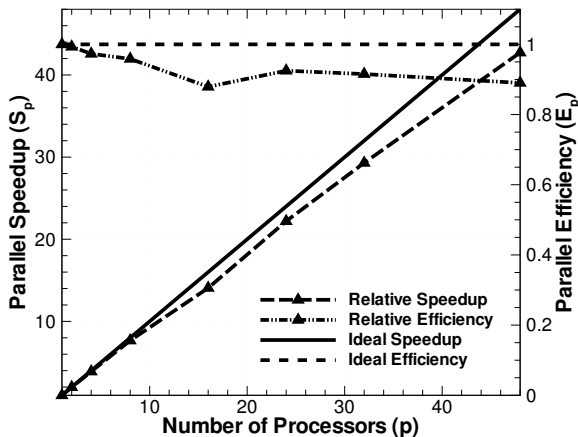
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Newton-Krylov Convergence



Non-Premixed Laminar Diffusion Flame

Parallel Performance with 96 blocks



Parallel Speedup $S_p = t_1/t_p$, Parallel Efficiency $E_p = S_p/p$

Improved LES Capabilities

Grid-Independent LES

- ▶ explicit discrete filtering, adaptive mesh refinement (AMR)
- ▶ allow assessment and validation of subfilter scale models

High-Order Finite Volume Schemes

- ▶ high-order central essentially non-oscillatory (CENO) solution reconstruction (Ivan & Groth, 2006)
- ▶ parallel implementation with AMR

Least-Squares Discrete LES Filters

- ▶ high-order commutative discrete filters based on least-squares solution reconstruction

Thickened Flame Model

Modified Species Transport Equations

$$\frac{\partial(\bar{\rho}\tilde{Y}_n)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{Y}_n\tilde{u}_j)}{\partial x_j} = -\frac{\partial(E\tilde{F}J_{j,n})}{\partial x_j} - \frac{\partial[E\tilde{F}\bar{\rho}(\tilde{Y}_n\tilde{u}_j - \tilde{Y}_n\tilde{u}_j)]}{\partial x_j} + \frac{E\bar{\omega}_n}{F}$$

$$D \rightarrow EF\bar{D}, \quad \mu \rightarrow FE\mu, \quad \dot{\omega} \rightarrow E\dot{\omega}/F$$

Power-Law Flame Wrinkling Model

$$\frac{s_{T\Delta}}{s_l^0} = \frac{A_{\text{sfs}}}{\Delta^2} = \Xi_{\Delta} = \left(1 + \frac{\Delta}{\eta_c}\right)^{\beta} = E, \quad \eta_c = |\langle \nabla \cdot \mathbf{n}_s \rangle|^{-1}$$

where E is the efficiency factor, Ξ_{Δ} is the subfilter wrinkling factor, and η_c is an inner cutoff scale

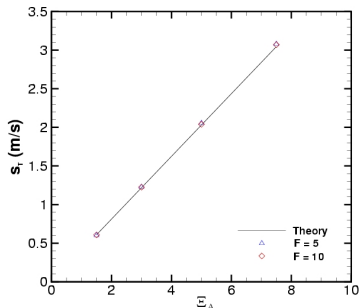
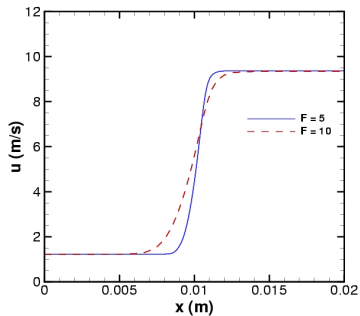
Thickened Flame Model

Efficiency Function (Charlette *et al.* , 2002)

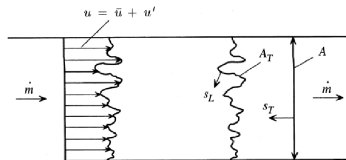
$$|\langle \nabla \cdot \mathbf{n} \rangle_s| = \Delta^{-1} \frac{u'_\Delta}{s_l^0} \Gamma \left(\frac{\Delta}{\delta_l^0}, \frac{u'_\Delta}{s_l^0}, Re_\Delta \right)$$

$$\Gamma \left(\frac{\Delta}{\delta_l^0}, \frac{u'_\Delta}{s_l^0}, Re_\Delta \right) = \{ [(f_u^{-a} + f_\Delta^{-a})^{-1/a}]^{-b} + f_{Re}^{-b} \}^{-1/b},$$

Thickened Flame Structure

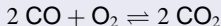
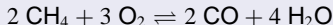


Freely Propagating Methane/Air Flame



Chemical Kinetic & Thermodynamic/Transport Models

- ▶ 2-step 6-species reduced chemical kinetic scheme (Westbrook & Dryer, 1981):



- ▶ thermodynamic & transport properties (Gordon & McBride, 1994, 1996)
- ▶ mixture viscosity and thermal conductivity rules of Wilke (1950) and Mason & Saxena (1964)

Thickened-Flame/Powerlaw-Flame-Wrinkling Model Solutions

Parameters Characterizing Premixed Flame:

$\phi = 1$, $\bar{u} = s_l^0$, $u' = 2.53$ m/s, $\ell = 7.3$ mm, $\lambda = 1.34$ mm,
 $Re_\ell = 1164$, $Re_\lambda = 213$, $s_l^0 = 0.406$ m/s, and $\delta_l^0 = 0.27$ mm.

Calculations Performed in Three Steps:

- ▶ 1D laminar flame solution
- ▶ Wrinkling of the flame front by 2D homogenous turbulence without reactions (Rogallo, 1981)
- ▶ 2D wrinkled flame front with reactions

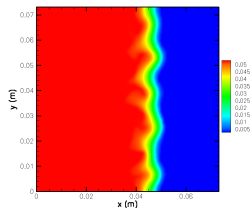
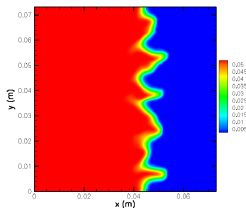
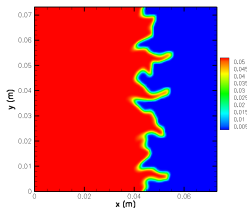
CH₄, $F = 10$

CH₄, $F = 5$

CO, $F = 10$

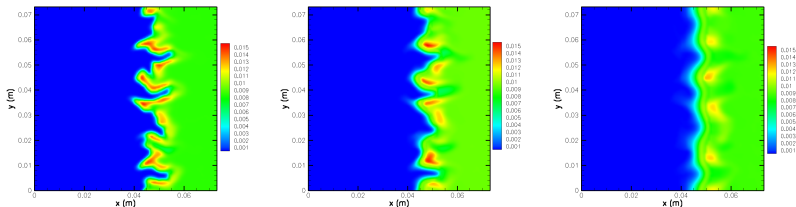
CO, $F = 5$

Predicted Turbulent Flame Structure



- ▶ Distributions of CH₄ mass fraction at $t = 0.98$ ms (after 2.8 eddy turnover times)
- ▶ $F = 5, 10, 20$

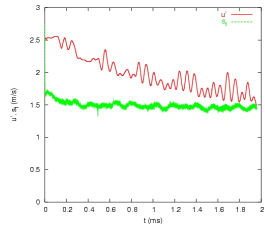
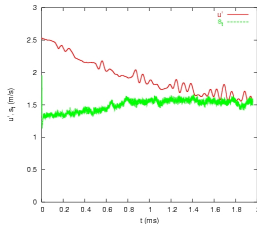
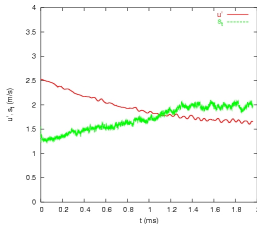
Predicted Turbulent Flame Structure



- ▶ Distributions of CO mass fraction at $t = 0.98$ ms (after 2.8 eddy turnover times)
- ▶ CO enhancement in positive cusps (Echekki & Chen, 1996; Hawkes & Chen, 2004)

Predicted Turbulent Burning Rate

Rate of consumption of methane: $s_t = \frac{1}{\rho_0 Y_0 L_y} \int_A \bar{\omega}_F dA$



Burning rate, $F = 5, 10, 20$

Gülder expression (1990)

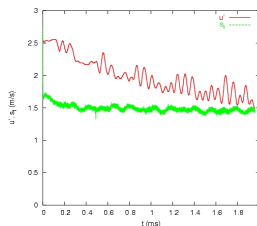
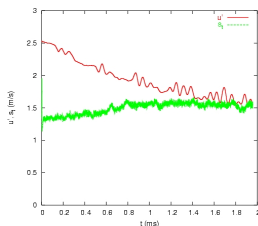
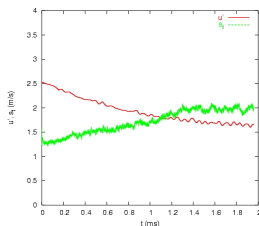
1.5 m/s

Average burning rate ($F=10$)

1.544 m/s

Predicted Turbulent Burning Rate

Rate of consumption of methane: $s_t = \frac{1}{\rho_0 Y_0 L_y} \int_A \bar{\omega}_F dA$



Burning rate, $F = 5, 10, 20$

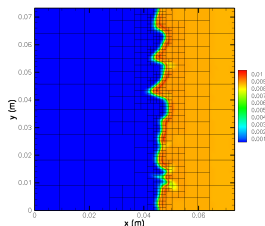
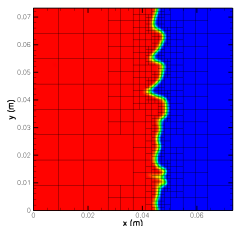
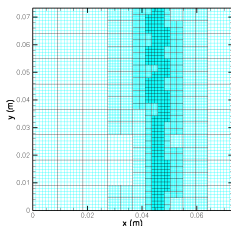
Gülder expression (1990)

1.5 m/s

Average burning rate ($F=10$)

1.544 m/s

Predicted Turbulent Flame Structure Using AMR



- ▶ Computational mesh and distributions of CH₄ and CO mass fractions at $t = 0.245$ ms
- ▶ 4 levels of mesh refinement, 8×8 solution blocks, 600-700 blocks

Flame Surface Density (FSD) SFS Model

The flame surface density (FSD) model of Hawkes and Cant (2000, 2001) is being developed for predicting premixed combustion via LES

$$c = \frac{T - T_u}{T_b - T_u} \quad \text{or} \quad c = \frac{Y_F - Y_F^u}{Y_F^b - Y_F^u} \quad 0 \leq c \leq 1$$

$$\frac{\partial}{\partial t} (\rho \tilde{c}) + \frac{\partial}{\partial x_i} (\rho \tilde{u}_i \tilde{c}) + \frac{\partial}{\partial x_i} \rho (\tilde{u}_i \tilde{c} - \tilde{u}_i \tilde{c}) = \frac{\partial}{\partial x_i} \left(\overline{\rho D \frac{\partial c}{\partial x_i}} \right) + \bar{\dot{\omega}}_c = \overline{\rho s_d |\nabla c|}$$

$$\overline{\rho s_d |\nabla c|} \approx \rho_u s_L \Sigma$$

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial}{\partial x_i} (\tilde{u}_i \Sigma) = - \frac{\partial}{\partial x_i} (\overline{(u_i)_s'} \Sigma) + (S_{mean} + S_{hr} + S_{sg}) \Sigma + P_{mean} + P_{sg}$$

G-Equation SFS Model

A G-equation approach is being developed for predicting premixed combustion via LES. Assumes thin flame surface and flame-front position is represented with a constant value of the level set function, G (Williams, 1985; Kerstein & Williams, 1988; Peters, 2000; Pitsch & Duchamp de Lageneste, 2002).

$$\frac{\partial(\bar{\rho}\tilde{G})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{G})}{\partial x_i} = \overline{\rho w |\nabla G|}$$
$$w = \bar{s}_T \quad \frac{\bar{s}_T}{s_L} = 1 + \alpha \left(\frac{\bar{u}'}{s_L} \right)^q$$

Concluding Remarks

- ▶ Overview of numerical modelling of premixed combustion processes: motivation, numerical challenges, and approaches
- ▶ Described numerical results for thickened-flame/powerlaw-flame-wrinkling model
- ▶ Future Research
 - ▶ Moving to three-dimensional turbulence
 - ▶ Comparison of subfilter scale models
 - ▶ Use of high-order spatial and temporal discretizations
 - ▶ Use of explicit filtering based on high-order commutative discrete filters
 - ▶ Study of hydrogen enrichment of methane

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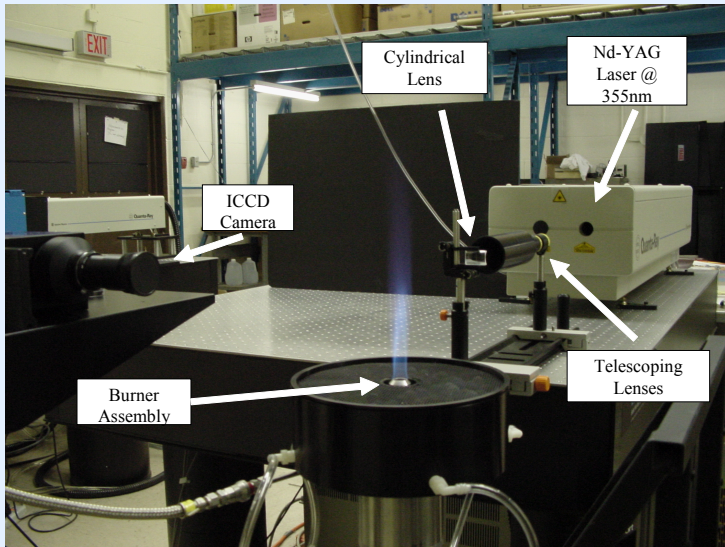
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Flame and Flow Parameters

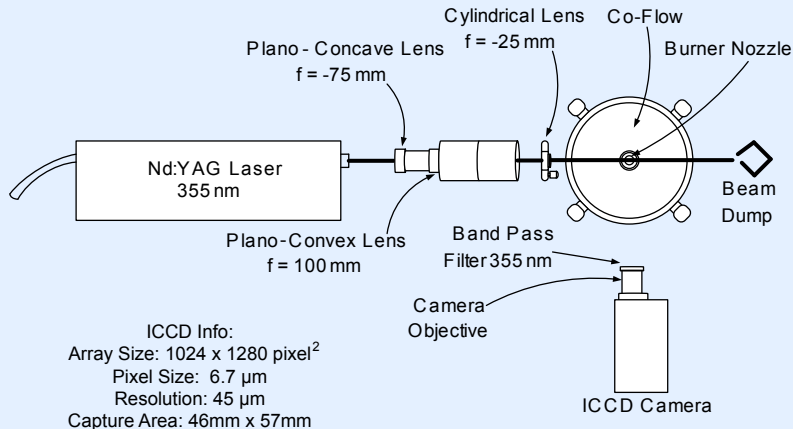
- Axisymmetric Bunsen-type burner
 - nozzle diameter of 11.2mm
 - turbulence was generated by perforated plates 3-diameter lengths upstream of the burner nozzle.
- Methane/air mixtures were selected to provide:

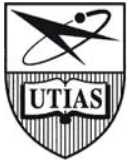
Exit velocities	14.43, 14.62, 14.77 m/s
Turbulent intensities (u')	1.37, 1.41, 1.81 m/s
Equivalence ratios (ϕ)	0.6, 0.7, 0.8, 0.9, 1.0
Non-dimensional turbulent intensities (u'/S_L)	3.4 - 15.3

Planar Rayleigh Scattering Setup

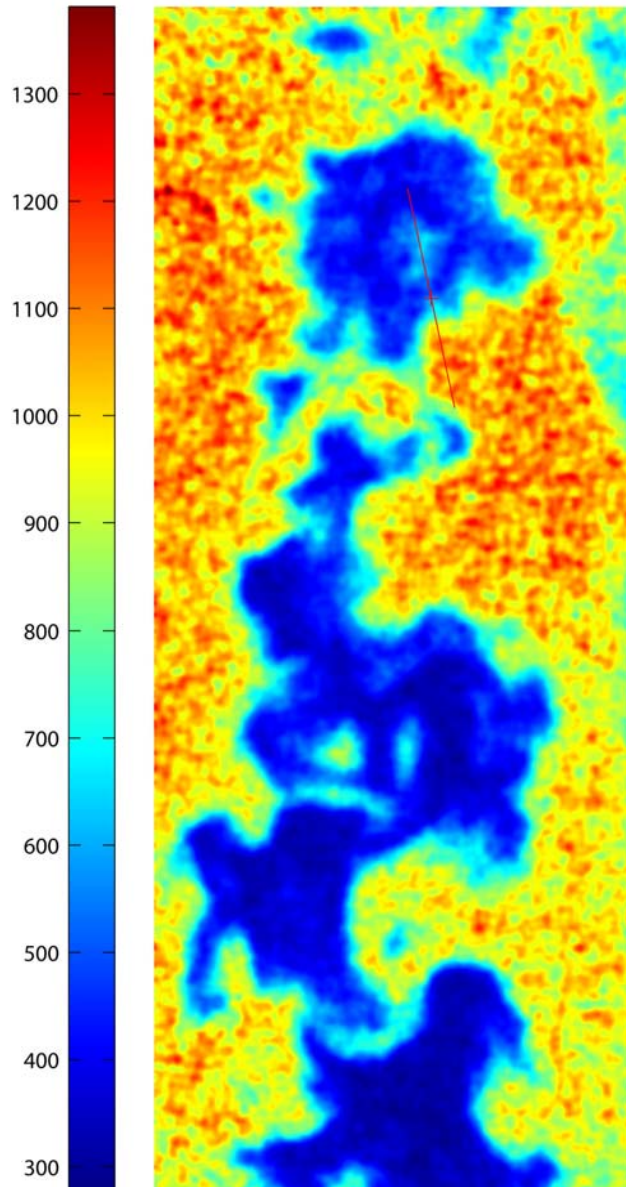


Planar Rayleigh Scattering Setup

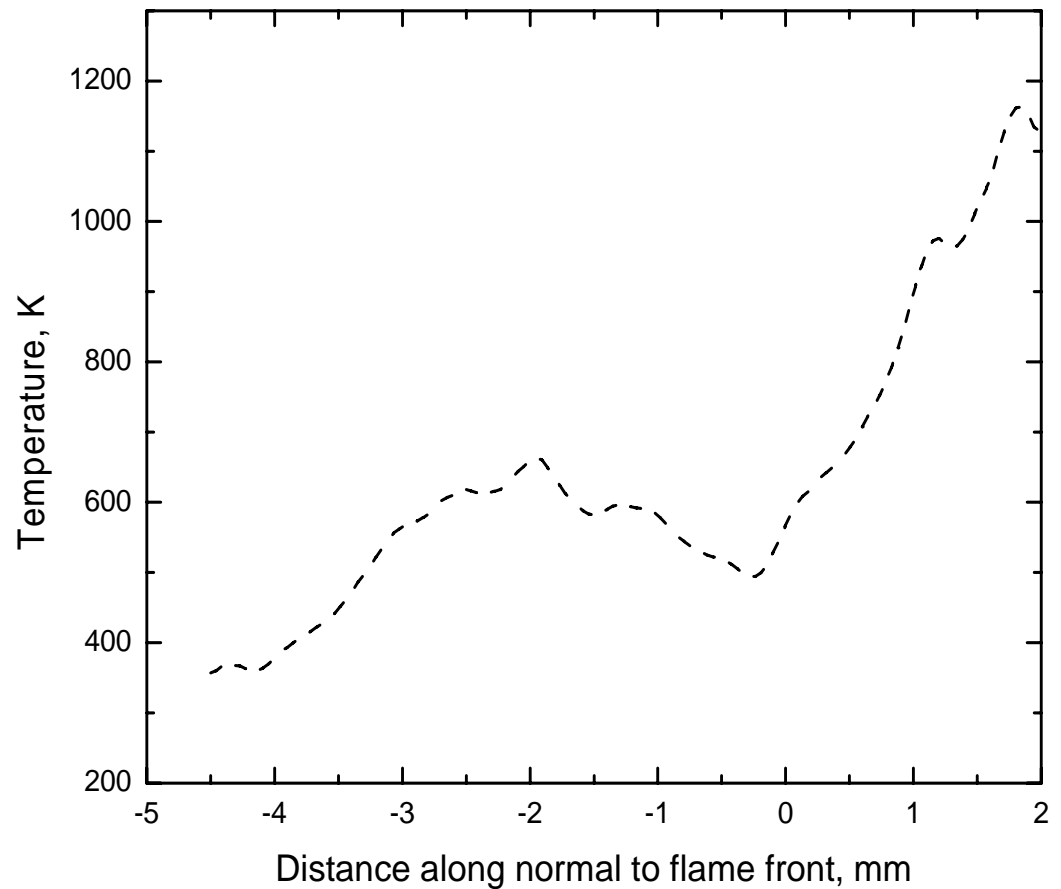


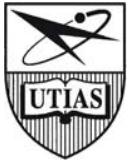


Flame Front Temperature

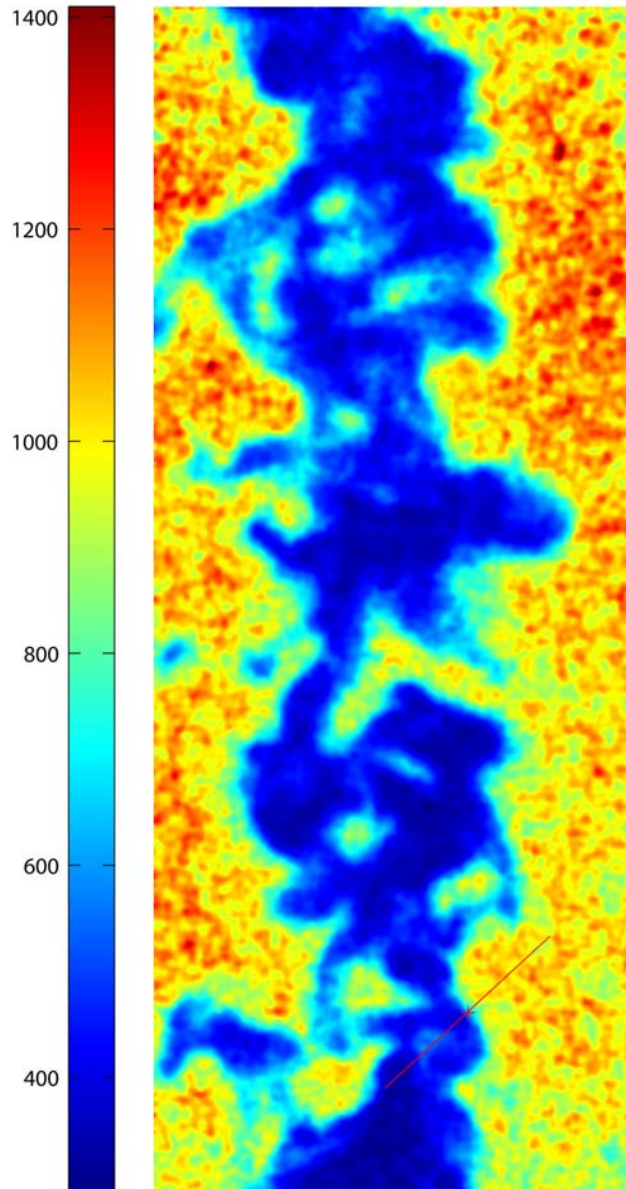


Rayleigh scattering; CH₄-air
 $\Phi = 0.7$; $u'/S_L = 15$

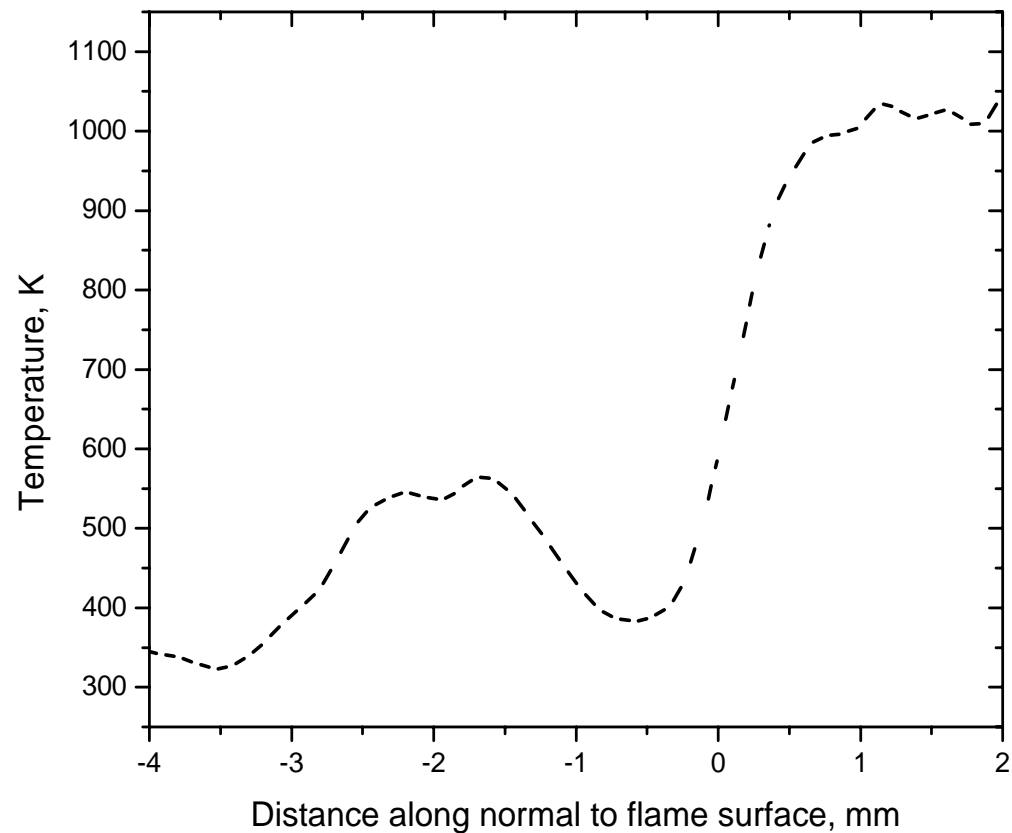


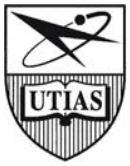


Flame Front Temperature

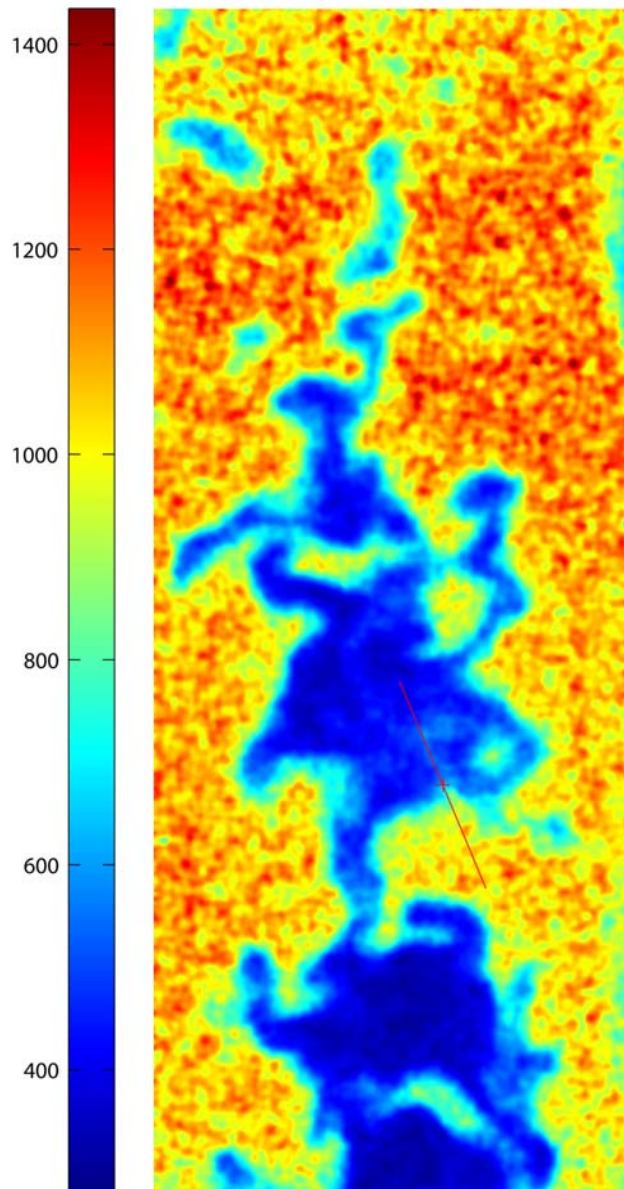


Rayleigh scattering; CH₄-air
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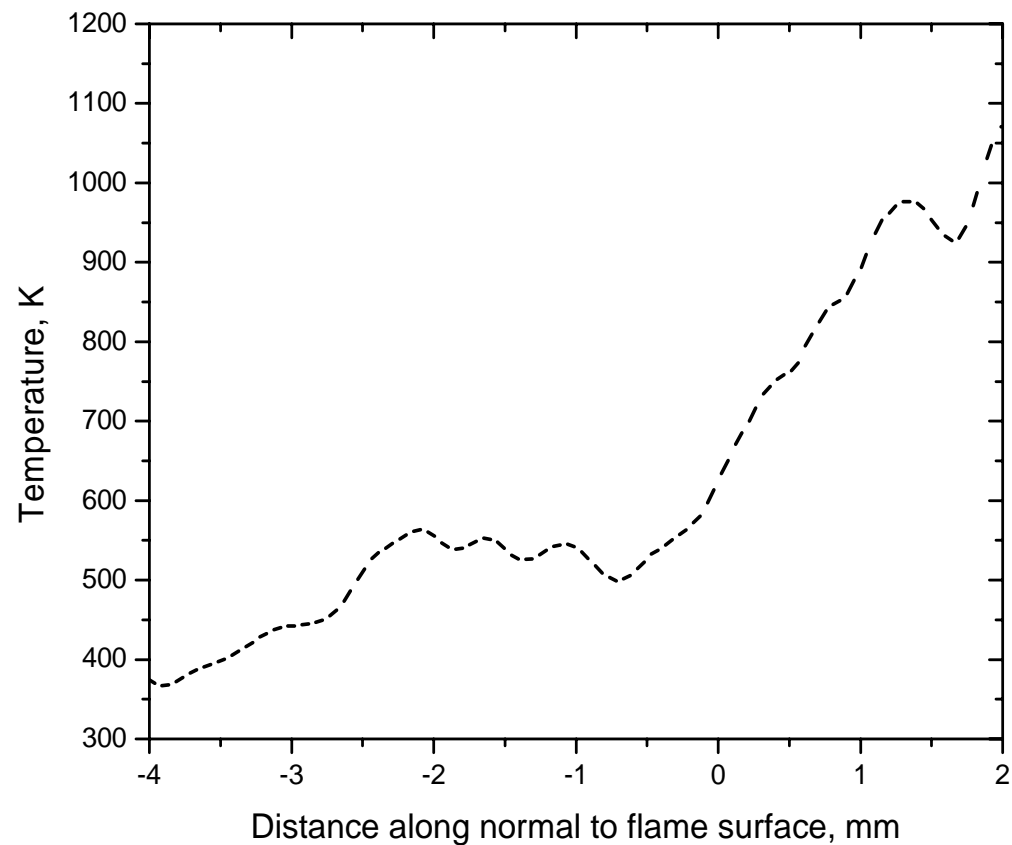


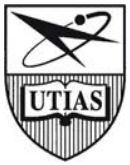


Flame Front Temperature

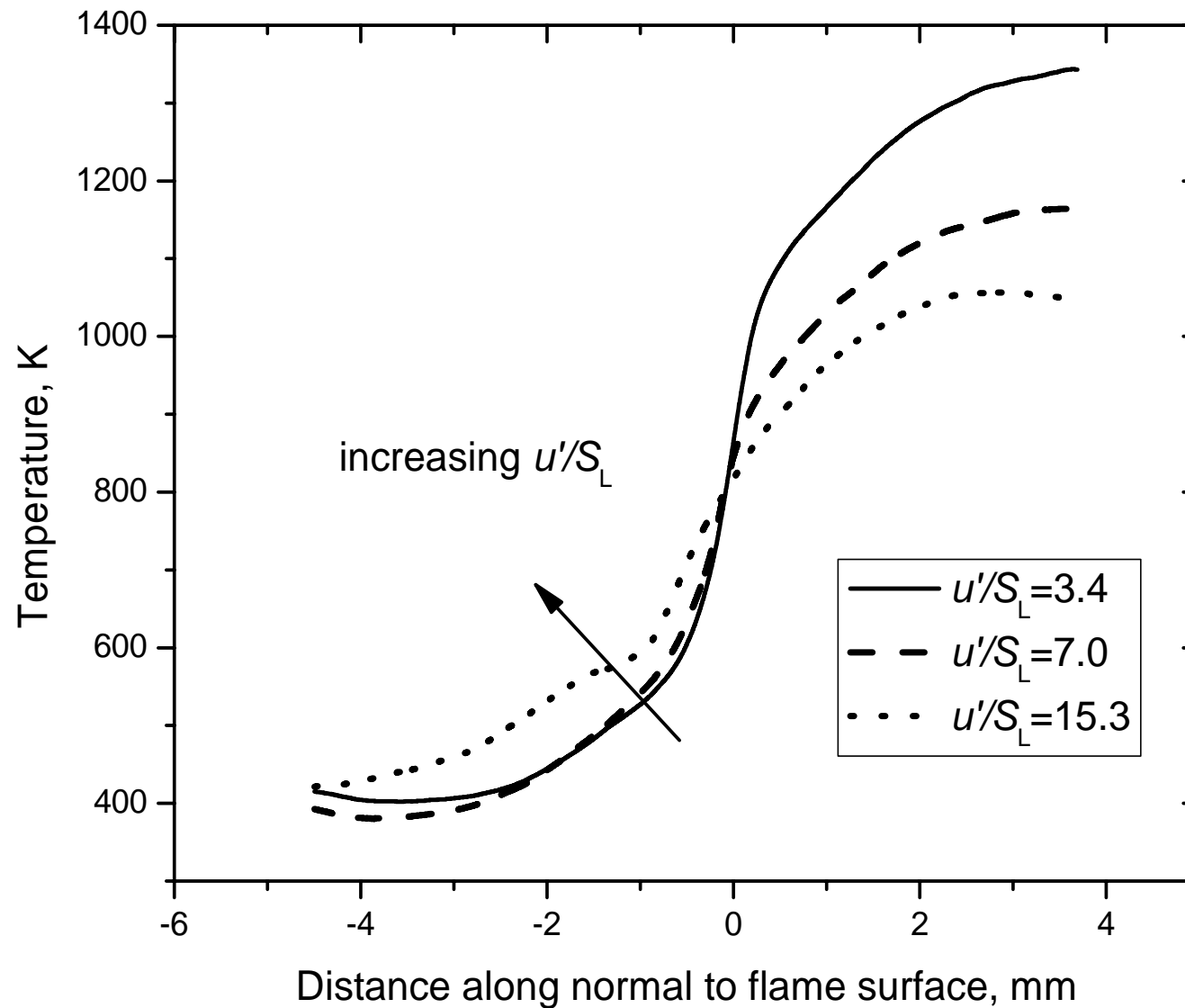


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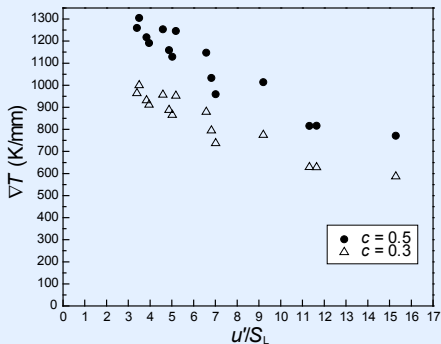




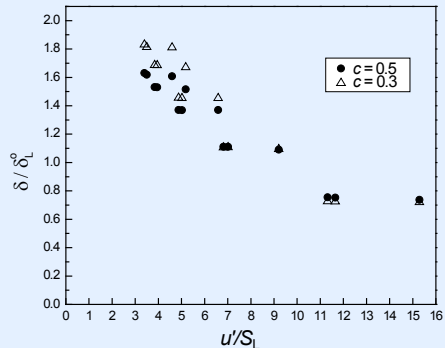
Averaged Temperature Profiles



Effects of Non-Dimensional Turbulent Intensities

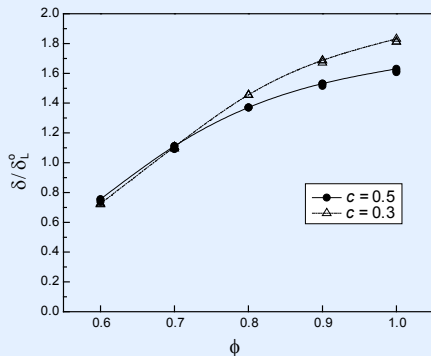


Variation of Gradients with u'/S_L

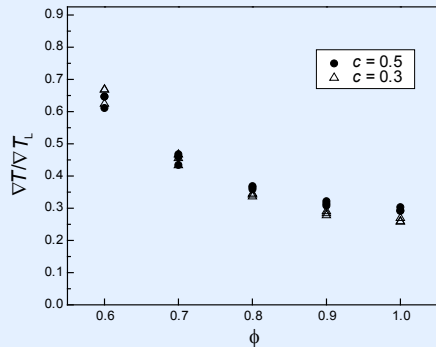


Normalized flame front thicknesses by unstretched laminar flame thickness (δ_L^0) at different u'/S_L

Effect of Equivalence Ratio



Normalized flame front thickness as a function of equivalence ratio (ϕ)



Normalized temperature gradients as a function of equivalence ratio (ϕ)



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Flammability Limit and NO_x Formation of Fuel Enriched Lean Premixed Flames

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National Research
Council Canada

Conseil national
de recherches Canada

Canada

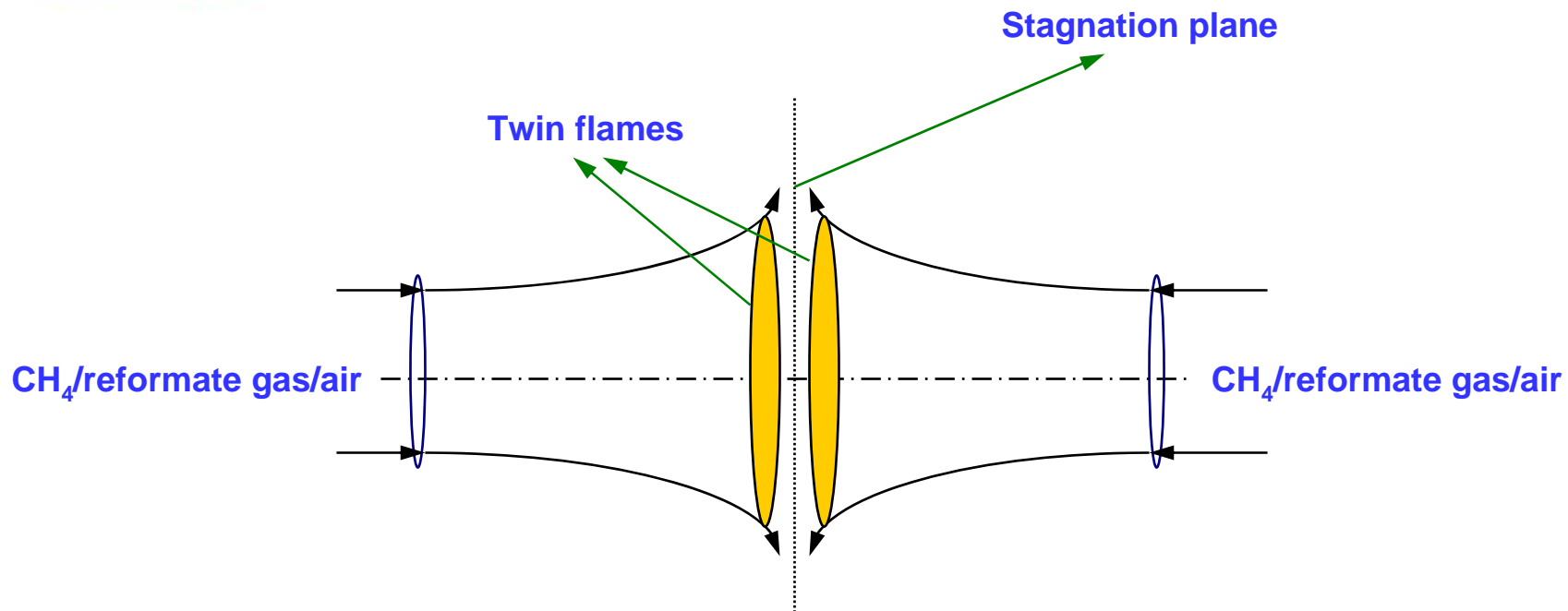
Background

- Lean premixed combustion is a promising concept for significantly improving fuel conversion efficiency and reducing pollutant emissions;
- Lean premixed flames are less stable, due to the narrow flammable range at leaner condition;
- Hydrogen enrichment can enlarge the flammable range of lean premixed flames, and thus improve flame stability;
- Hydrogen can be obtained by fuel reforming;
- A reformat gas contains not only hydrogen, but also carbon monoxide and other components;
- ***Will reformat gas enrichment be helpful?***

Objectives

- Investigate the effect of reformat gas enrichment on extinction characteristics of CH_4 /air premixed flames;
- Study the mechanisms of NO_x formation in reformat gas enriched CH_4 /air lean premixed flames.

Flame Configuration



Numerical Model

- Potential boundary conditions;
- Adaptive refinement of meshes;
- Atmosphere pressure, and room temperature, 300 K;
- Radiation: optically thin model;
- Reaction scheme: Gri-Mech 3.0;
- Reformate gases: partial oxidation of CH₄

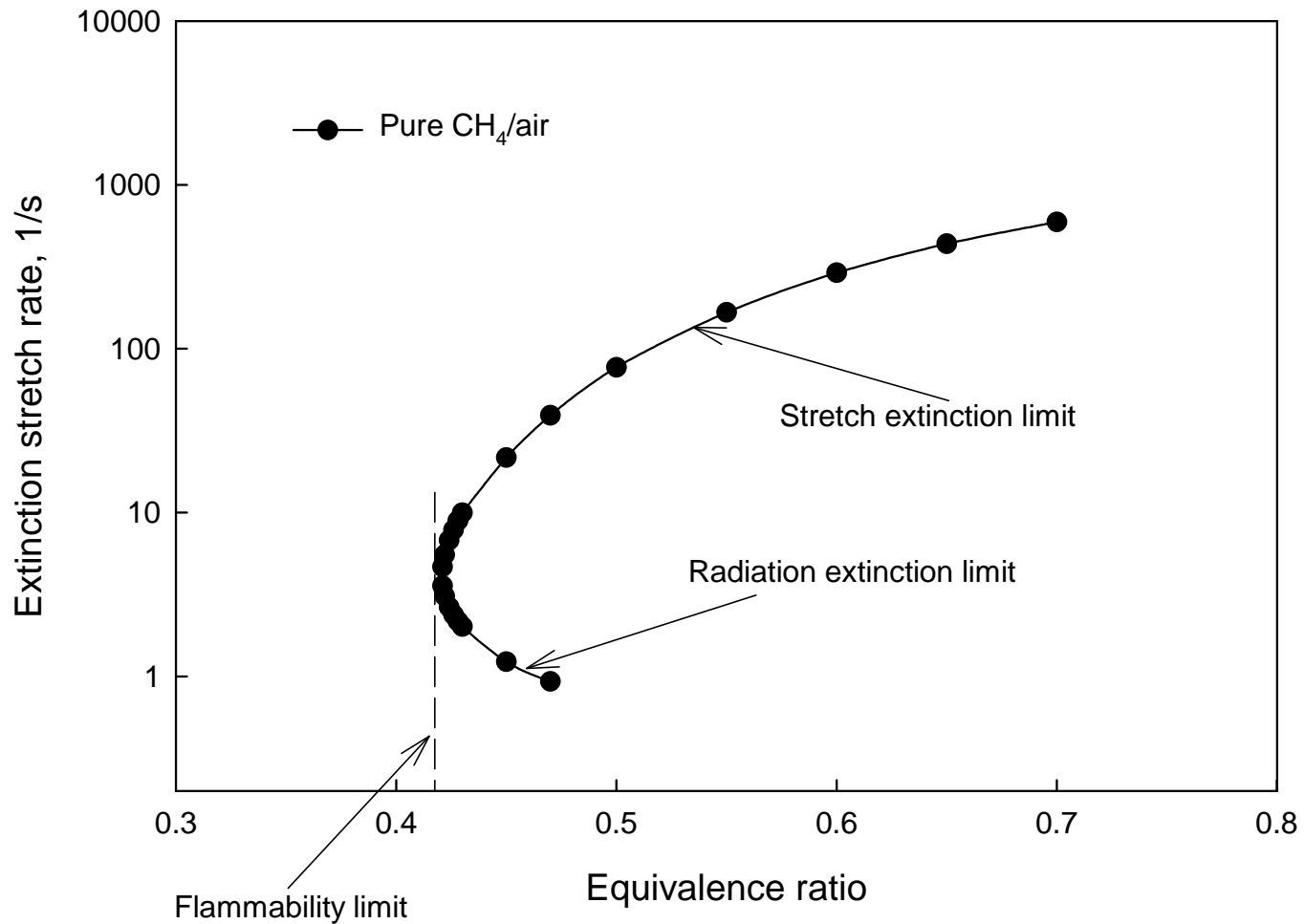


$\gamma = 0$ --- reformate gas 1

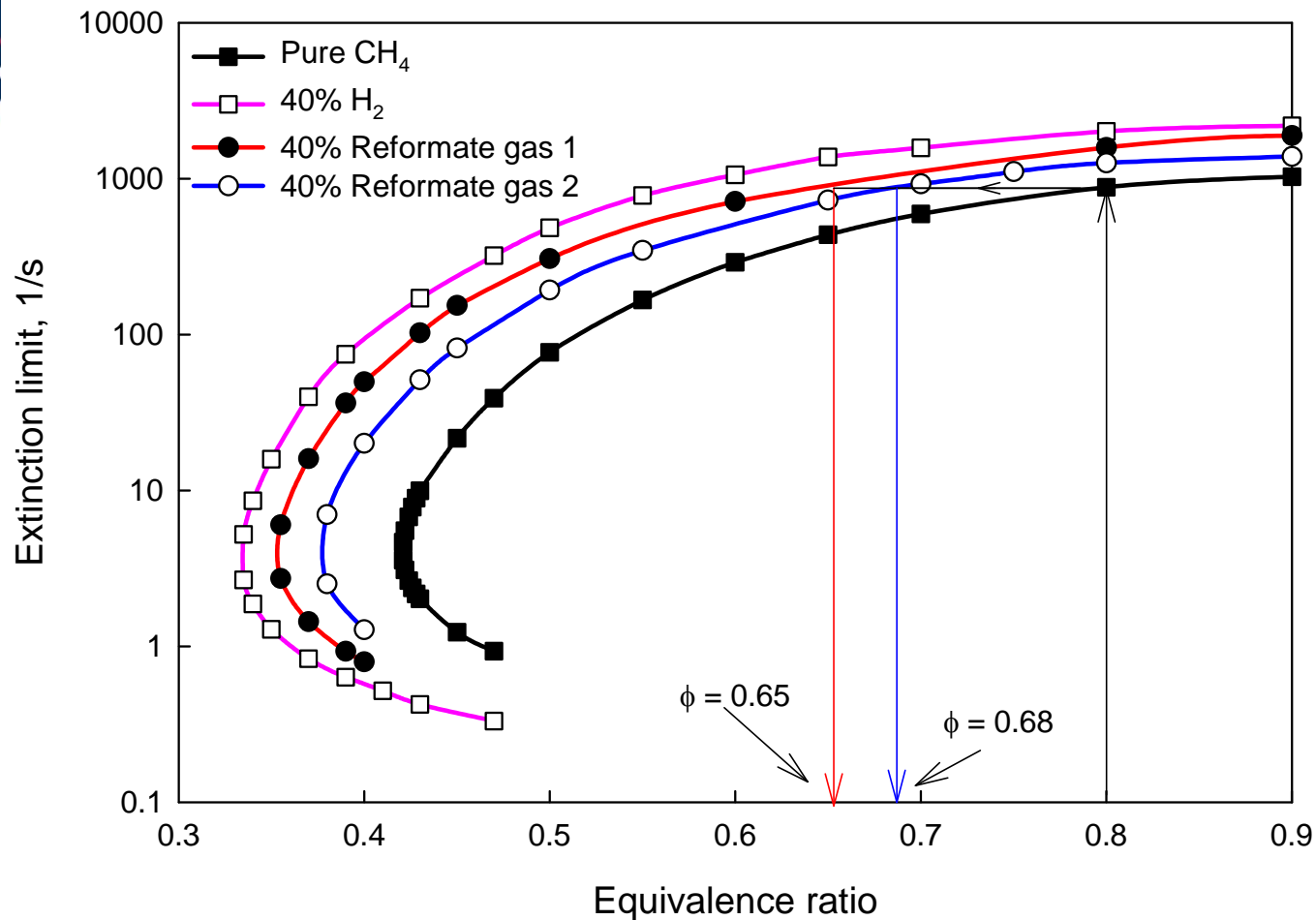
$\gamma = 3.76$ --- reformate gas 2

Enrichment fraction: $\alpha_{\text{rg}} = V_{\text{rg}} / (V_{\text{rg}} + V_{\text{CH}_4})$

Extinction Limits of Pure CH₄/Air Flames



Extinction Limits

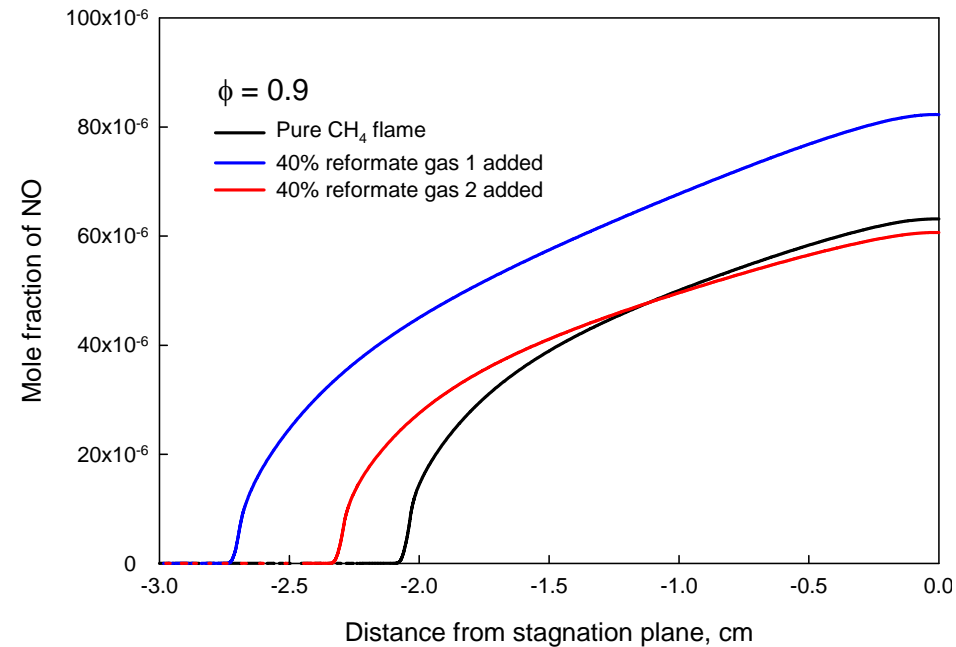
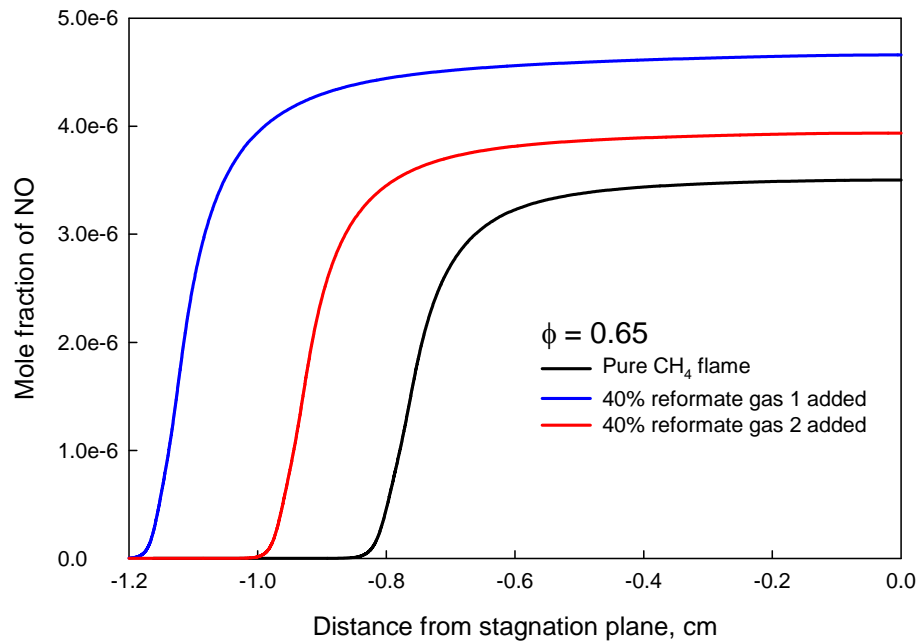


The addition of a reformate gas does enlarge the flammable range and lower the flammability limit.

NO Formation

$$\phi = 0.65$$

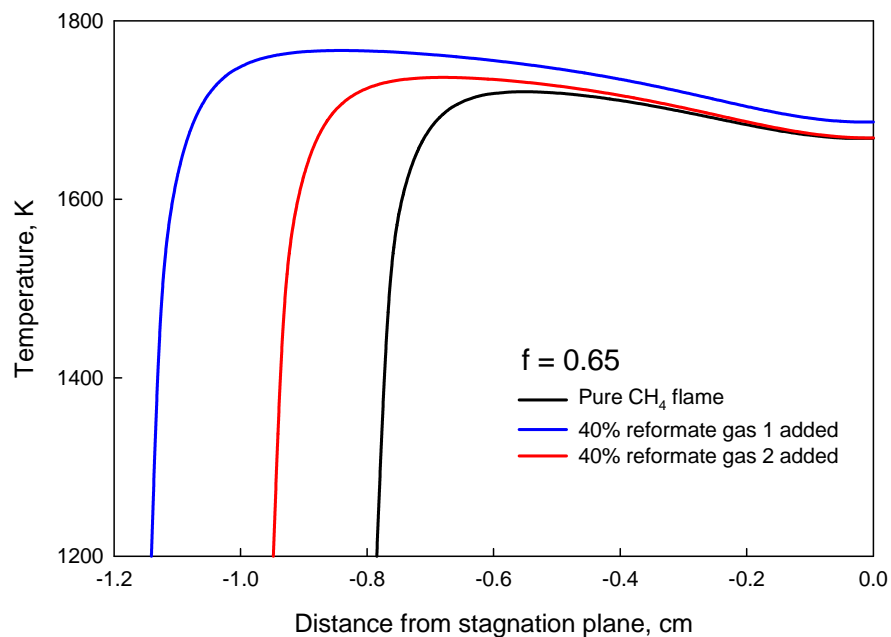
$$\phi = 0.9$$



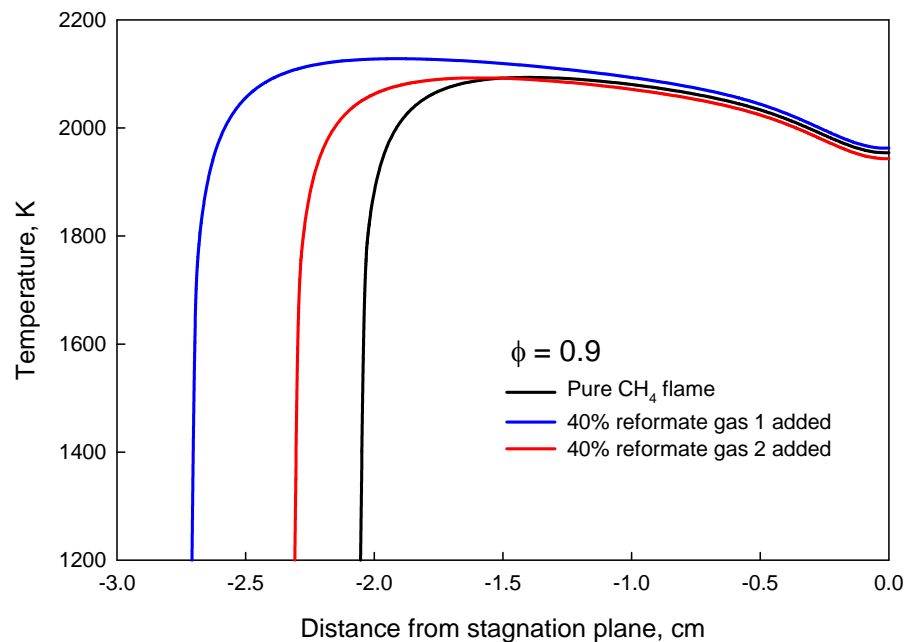
- The addition of reformat gas 1 always increases the formation of NO;
- The effect of reformat gas 2 addition on NO formation depends on equivalence ratio, because of the variation in flame temperature.

Flame Temperature

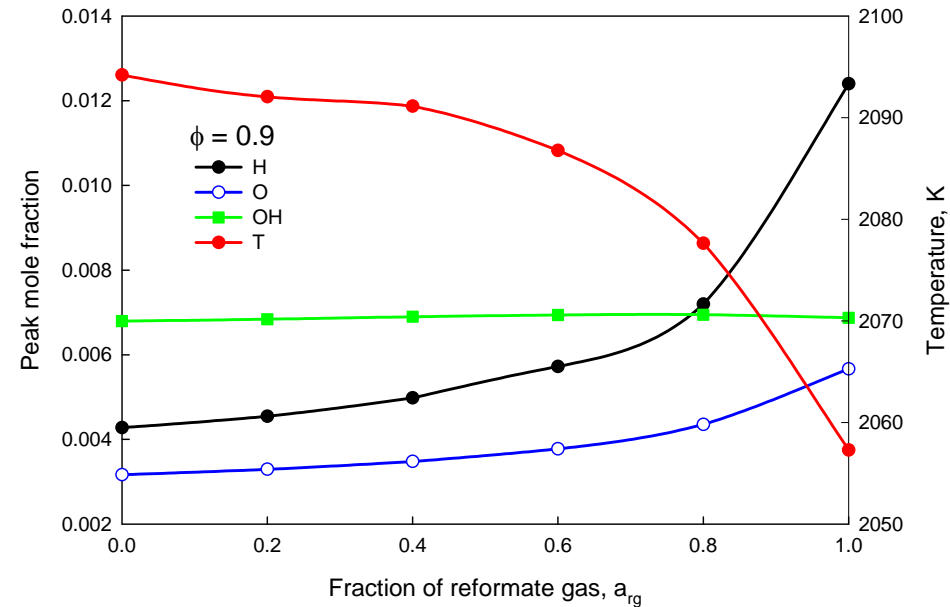
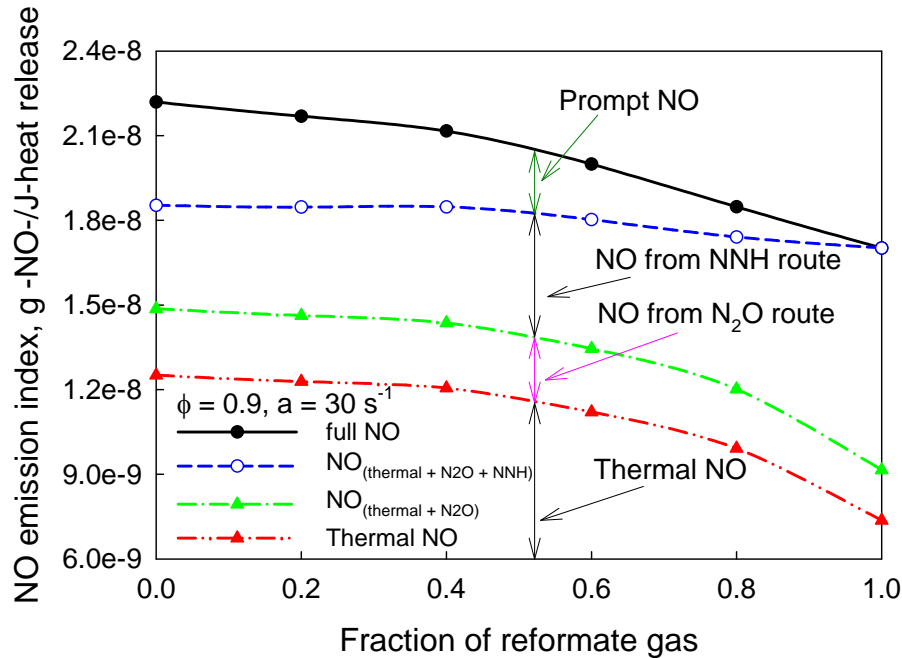
$\phi = 0.65$



$\phi = 0.9$

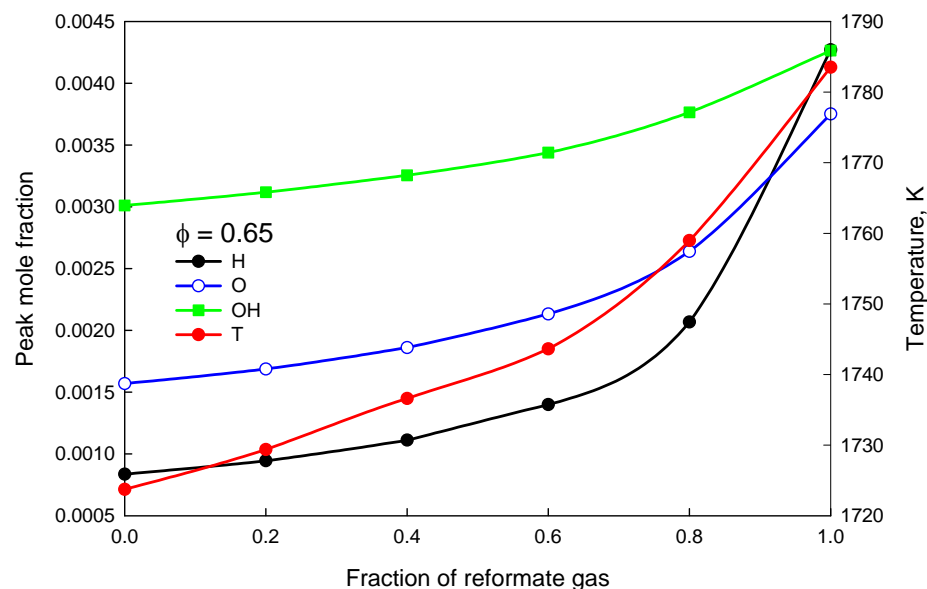
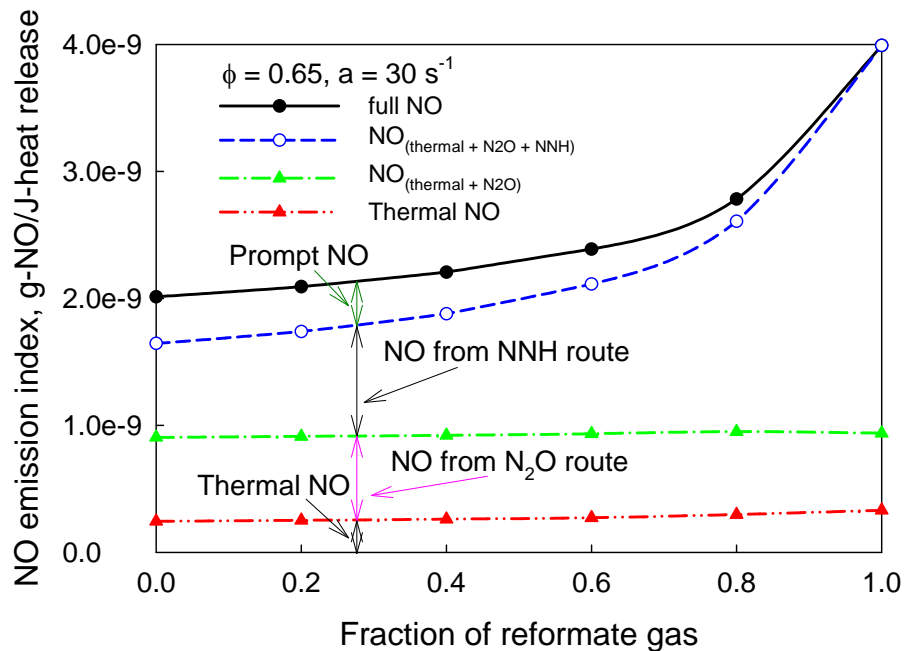


Variation of NO Formation Mechanism ($\phi = 0.9$, reformate gas 2)



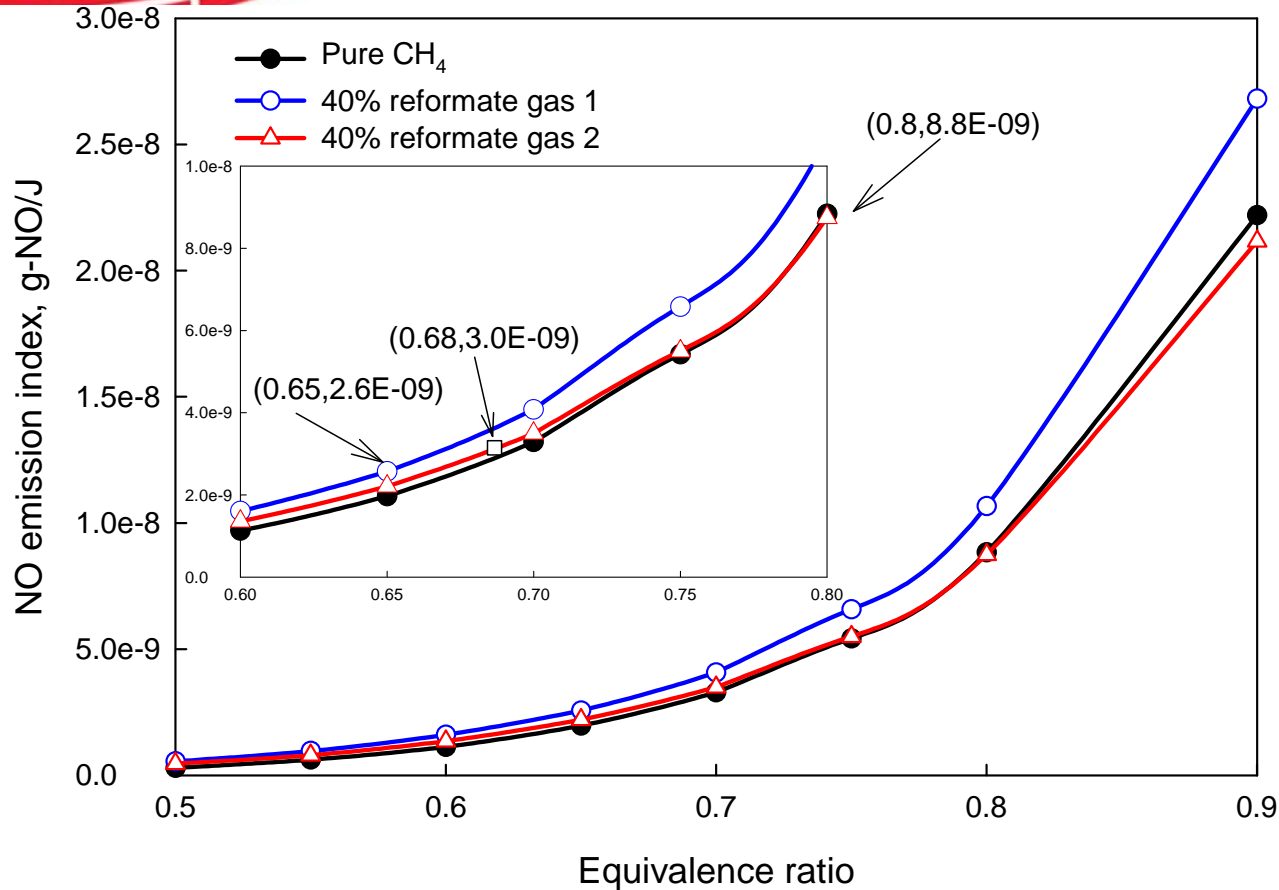
- The addition of reformate gas reduces the contributions of the prompt and thermal routes, because of the decrease in CH concentration and flame temperature;
- The contribution of the NNH intermediate route increases, because: $\text{NNH} = \text{N}_2 + \text{H}$, $\text{OH} + \text{H}_2 = \text{H}_2\text{O} + \text{H}$, $\text{CO} + \text{OH} = \text{H} + \text{CO}_2$.

Variation of NO Formation Mechanism ($\phi = 0.65$, reformat gas 2)



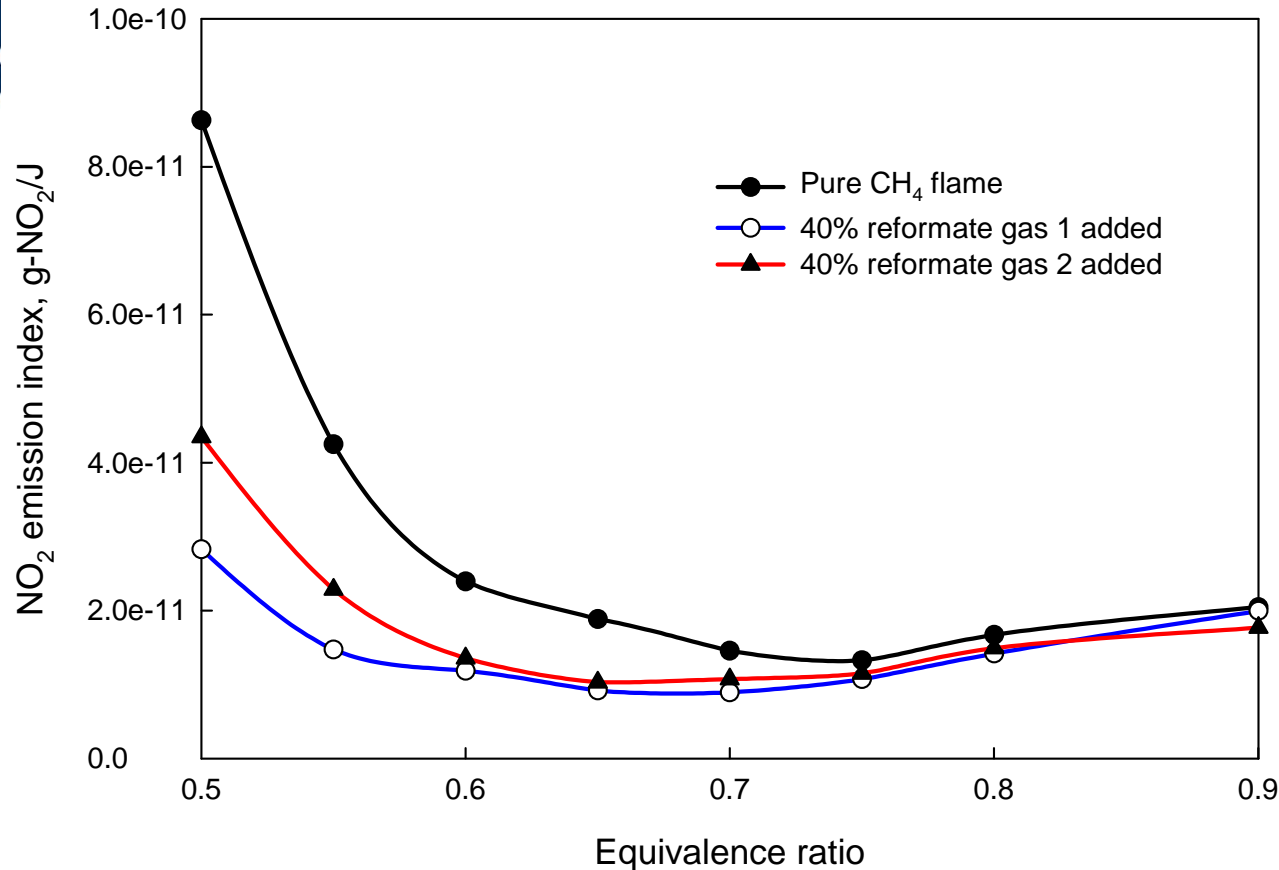
- Reformat gas addition significantly increases the contribution of the NNH route and slightly increases that of the thermal route;
- But reformat gas addition reduces the contribution of the prompt route.

NO Formation



- The formation of NO can be significantly reduced in a reformed gas enriched flame, by operating under leaner condition.

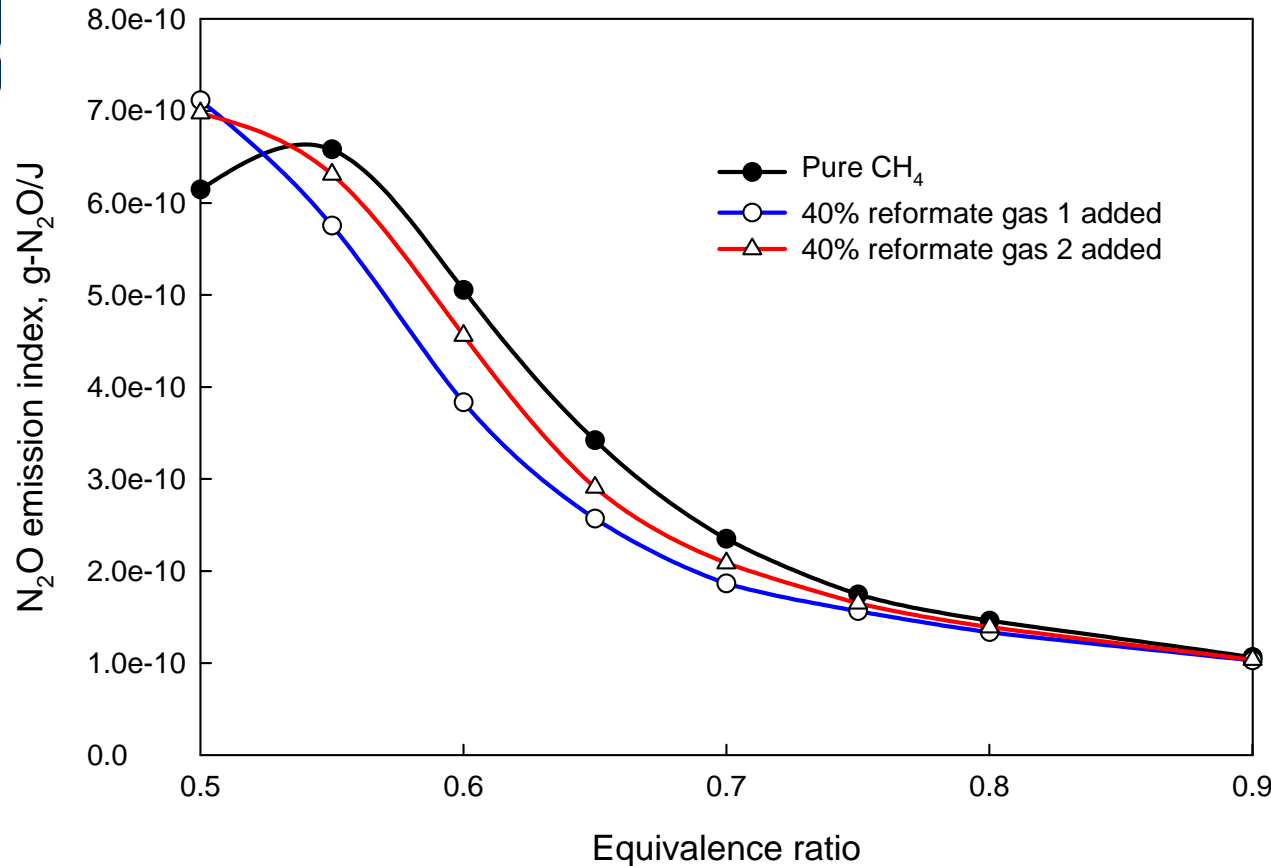
NO₂ Formation



- $\text{HO}_2 + \text{NO} = \text{NO}_2 + \text{OH}$
- $\text{NO}_2 + \text{H} = \text{NO} + \text{OH}$

- At a lower equivalence ratio, the addition of a reformat gas reduces the formation of NO₂, with the addition of reformat gas 1 being more effective;
- At $\phi = 0.9$, the addition of reformat gas 2 is more effective to reduces the formation of NO₂ than that of reformat gas 1.

N₂O Formation



- $\text{N}_2\text{O} (+\text{M}) = \text{N}_2 + \text{O} (+\text{M})$
- $\text{N}_2\text{O} + \text{H} = \text{N}_2 + \text{OH}$

- At a constant ϕ , the addition of a reformat gas reduces the formation of N₂O, because of the increase in the N₂O destruction rate;
- At a constant enrichment fraction, the formation of N₂O increases with the decrease of equivalence ratio, except for the flame close to extinction.

Conclusions

- The addition of a reformat gas enlarges the flammable range and lowers the flammability limit of stretched lean CH_4 /air premixed flame;
- The reformat gas enrichment allows a combustor to operate at leaner condition;
- Although the addition of a reformat gas may increase the formation of NO at a constant equivalence ratio, it can significantly reduce the emission of NO by allowing a combustor to operate under leaner condition;
- At a leaner operating condition, the formation of NO_2 and N_2O relatively increases. However, the addition of a reformat gas can moderate this effect.



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