CCC Annual Report

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Modeling SEN Preheating with FLUENT and GASEQ

Yonghui Li

Department of Mechanical Science & Engineering

University of Illinois at Urbana-Champaign

Project Background (long term goals)

- SEN Preheating ⇨ Prevent thermal shock cracks
- Cool down process ⇨ Transport the preheated SEN
- Initial Casting Immersion ⇨ Possible skulling in mold and associated defects
- 3D commercial software model ⇨ Long time& expansive

⇨ 1D User friendly Visual Basic Application

Flame Temperature VBA Model predicts flame temperature, convection coefficients etc. in preheating.

Heat Transfer VBA Model predicts SEN temperature histories during preheating, cool-down and casting.

Experiment: preheating experiment photo[1]

Temperature is measured here, the flame temperature measurement is at this axial level, which is 394mm in x-coordinate in FLUENT mode.

Model Approach

Combustion, Fluid flow, and Heat Transfer in and near Nozzle with 2-D axisymmetric FLUENT model

Post processing to get air entrainment, temperature distribution, heat transfer coefficients

Given air entrainment, Gaseq outputs flame temperature, heat transfer coefficients

Transient Heat Transfer VBA Model of nozzle predicts temperature histories

Mixture composition and mass flow rate

Gas flow data [1]

All Runs	Flow rate (SCFM)	Flow rate (m^3/s)	Gage Pressure(PSI)	Gage Pressure (kPa)
Oxygen	**6**	$6.972*10^{-4}$	**45**	310.30
Gas(CH_4)	**7.5(wrong, not use)**	$2.195*10^{-3}$	**9**	62.06

Experimental conservation

$\dot{n}_{CH4}/\dot{n}_{O2} = 1/2$

Blue flame color ⇨ **Complete combustion** High temperature ⇨ Assume pressures and O2 flow rate (less total flow rate) measured accurate

Suspect measured flow rates Less accurate than the pressures ⇨

$$\dot{V}_{CH4} = \frac{\dot{n}_{CH_4} P_{O_2} T_{CH_4} \dot{V}_{O_2}}{\dot{n}_{O_2} P_{CH_4} T_{O_2}} = \frac{1(310300 + 101325) \times 293.15 \times 6.972 \times 10^{-4}}{2(62060 + 101325) \times 293.15} = 8.782 \times 10^{-4} m^3/s$$

$$\dot{n}_{O2} = \frac{P_{O_2} * \dot{V}_{O_2}}{R * T_{O_2}} = \frac{(310300 + 101325) * 6.972 * 10^{-4}}{8.314 * 293.15} = 1.177 \times 10^{-1} mole/s$$

$$\dot{m}_{total} = \dot{m}_{O_2} + \dot{m}_{CH_4} = \dot{n}_{O_2} * 32 + \dot{n}_{CH_4} * 16 = \boxed{4.709 \times 10^{-3} kg/s}$$

Mass flow rate at mixture inlet

Measurements[1] for model calibration

1. Measured gas temp (TC2) and refractory wall temperatures (TC3-6) (RUN2)

Thermocouple	TC2	TC3	TC4	TC5	TC6
X* (mm)	775	394	538	394	538
Y* (mm)	76	48	48	69	69
Temperature (°C)	1077	584	554	453	397

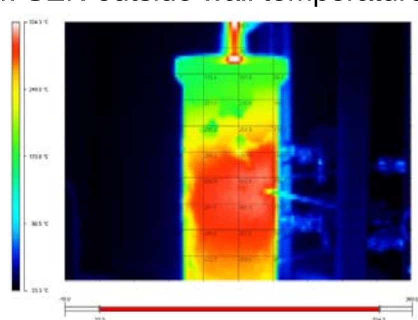
X: Distance from top air inlet;
Y: Distance from top air inlet.

2. Measured gas temperature across inner bore (X=394mm)

Distance from SEN center (mm)	0	5	10	15	20	25	30	35	40
Measured temperature (°C)	1432	1422	1403	1387	1337	1278	1204	1090	885

3. The shape of flame

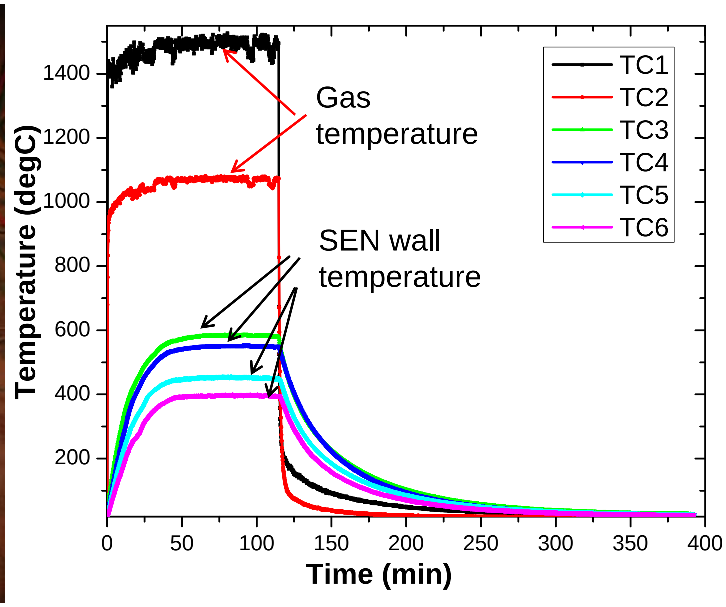
4. SEN outside wall temperature



Background: Torch preheating experiment for model validation

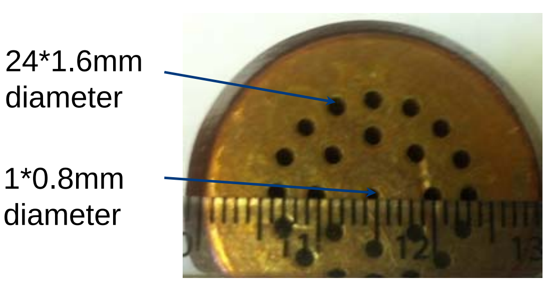
Set-up[1]

Thermal Couple temperature histories (Run2)

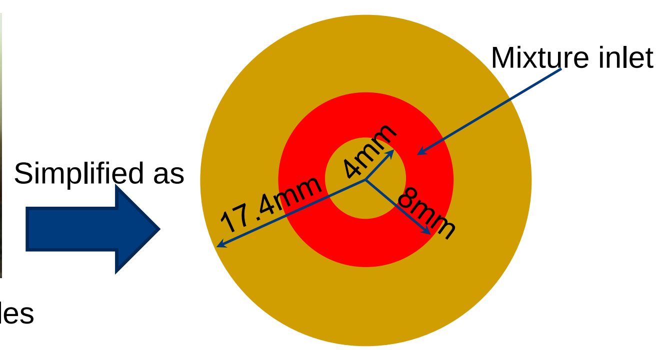


Model assumptions

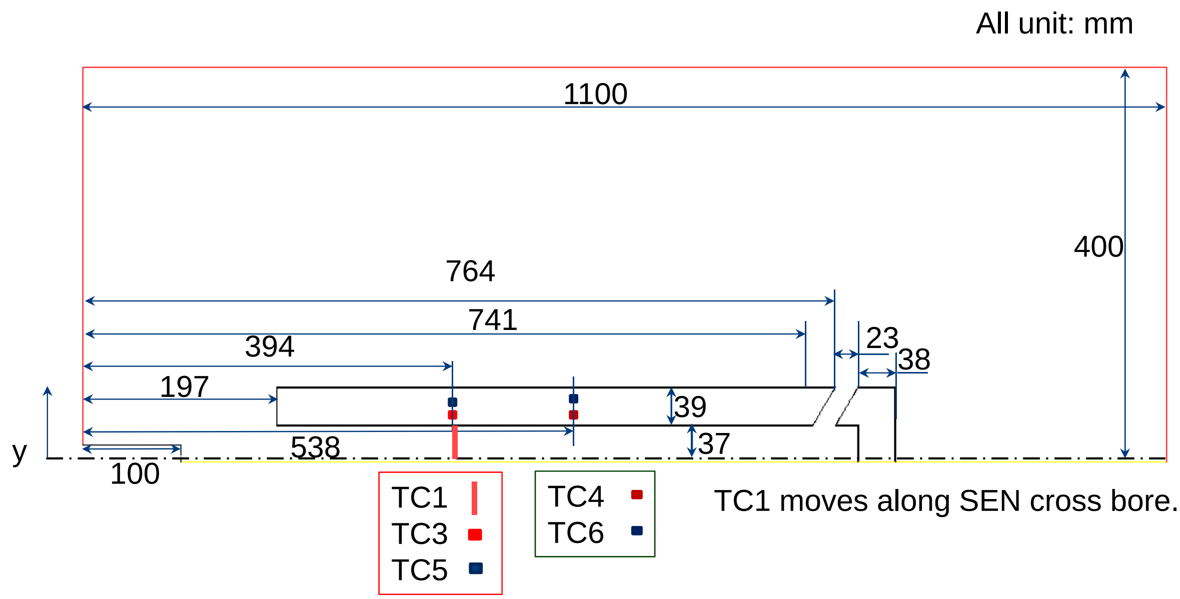
- FLUENT simulation is 2D asymmetric.
  - The two SEN ports are simplified as a ring shaped port with the same exit area.
- Assume the distance from the rosebud tip to where the combustion starts is very short, and can be neglected in the fluid flow model. So the temperature at the edge between the flowing gas and where combustion starts is 3105°C and the absolute pressure is 1atm.
- The rosebud tip is simplified as annular ring as following.



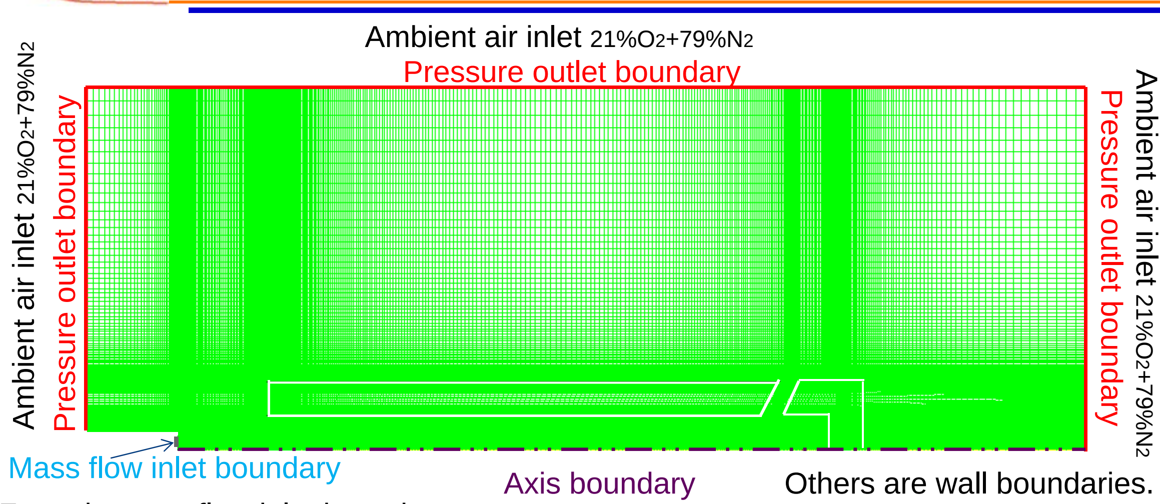
17.4mm diameter of outer ring of holes



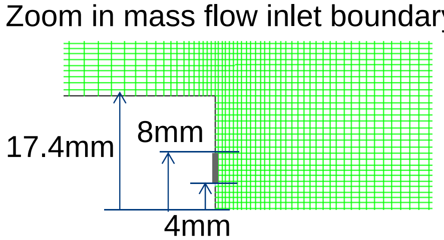
Model domain showing location of thermocouples



Simulation domain and mesh[2]



Zoom in mass flow inlet boundary



1-mm coating layer with 4 cells through thickness (0.25mm each)

88843 quadrilateral cells total

Fluent Model Settings[3]

Model	Steady state, 2D Axisymmetric, 9.81m/s^2 gravity	
	Energy conservation, P1 radiation	
	Turbulence model: Standard k-epsilon Enhanced Wall Function	
	Non-premixed species model	**Chemistry:** Steady Flamelet State Relation, operating pressure 101325Pa, non-adiabatic, Import CHEMKIN Mechanism (GRI-Mech 3.0 CHEMKIN file[4] of natural gas combustion, FLUENT thermo.db file of gas-phase thermodynamic database)
		Boundary: (Mole fraction) Fuel (3104.67℃) 0.3333CH4, 0.6667O2 Oxid (26.85℃): 0.7899 N2, 0.2101 O2

Model Settings

Material	PDF, Specific heat: mixing law, Thermal conductivity 2.7006W/m K, Viscosity 9.32e-5 kg/m s [5], refractive index=1, scattering coefficient =0, wsggm-domain-based absorption coefficient.	Solid material setting in slide 16.
Solver	Pressure based solver	
Pressure Schemes	SIMPLE, Second Order Upwind	

Steady laminar flamelet approach models a turbulent flame brush as an ensemble of discrete. The advantage of the laminar flamelet approach is that realistic moderate non-equilibrium chemical kinetic effects can be incorporated into turbulent flames.

GRI-Mech 3.0 is an “optimized mechanism” database designed to model natural gas combustion, contains **325 reactions** and **53 species**.

K-epsilon Turbulence Model

	Case 1(default)*	Case 2[6]
Cmu	0.09	0.09
C1-Epsilon	1.44	1.44
C2-Epsilon	1.92	1.87
TKE Prandtl Number	1	1
TDR Prandtl Number	1.3	1.3
Energy Prandtl Number	0.85	0.7
Wall Prandtl Number	0.85	0.7
PDF Schmidt Number	0.85	0.7

* Recommanded by Nakod P. from Ansys technique support.

Reasons for ~3000°C Fuel Boundary Temperature

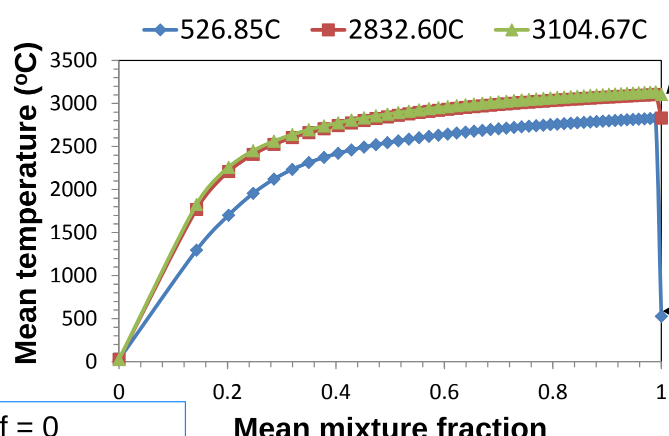
At fuel mixture inlet

$$\frac{\dot{n}_{CH_4}}{\dot{n}_{O_2}} = \frac{1}{2}$$

Stoichiometric combustion
Air entrains down the flame

⇨ Maximum temperature should be at fuel mixture inlet.

Result of 3104.67°C Fuel Boundary Temperature



Through iterations, mean temperature at f = 1 is assumed as 3104.67°C.

Result of 526.85°C Fuel Boundary Temperature

f = 0
Outlet (oxidant = air) boundary

f = 1
Fuel mixture inlet

Gas Mixture Properties

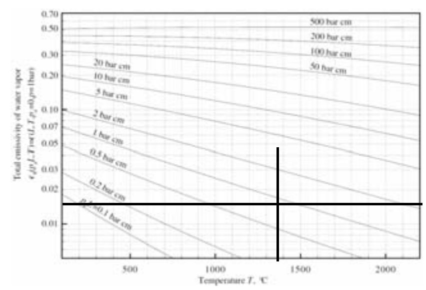
Emissivity

- Products partial pressure and flame temperature
  (Outputs from Gaseq)
  - With 100% oxygen source fraction and 151.96% air entrainment in 1atm and 27°C reactant temperature
- The complete combustion of CH_4 produces CO_2 and H_2O, which generate nonluminous radiation.
- The individual emissivity of CO2 and H2O can be looked up at the emissivity figures [7].
- The total emissivity can be calculated from Leckner [8] is 0.03.

Thermal conductivity and Viscosity

- Assume Ch4 (298K) adiabatically and stoichiometrically combusted with 95% O_2 and 5% N_2, the products equilibrium viscosity is 9.32×10^{-5} kg/ms and equilibrium thermal conductivity is 2.70 W/mK. [5]

Example: Emissivity of water vapor [7]



SEN (Solid) Material properties

Material	**Doloma Graphite**	
Density	2330 kg/m³	
Temperature(°C)	Thermal conductivity(W/m K)	Specific Heat (J/kg K)
25	26.5	750
500	21.8	1228
1000	17.7	1360
1500	14.6	1481

Material	**Glaze**	
Density	2000 kg/m³	
Emissivity	0.44 [9]	
Temperature(°C)	Thermal conductivity(W/m K)	Specific Heat (J/kg K)
25	0.90	821
200	1.20	1035
550	1.67	1281
1075	1.00	1611
1425	0.40	1836

Boundary conditions

Mass Flow Inlet

Mass flow rate (g/s)		4.709
Initial Gauge Pressure (Pa)		0
Turbulent Kinetic Energy (m^2/s^2)		0
Turbulent Dissipation Rate (m^2/s^3)		0
Temperature (℃)		3104.67
Mean Mixture Fraction Fuel		1
Mixture Fraction Variance		0
Radiation	Boundary temperature	
	Internal Emissivity	0.03

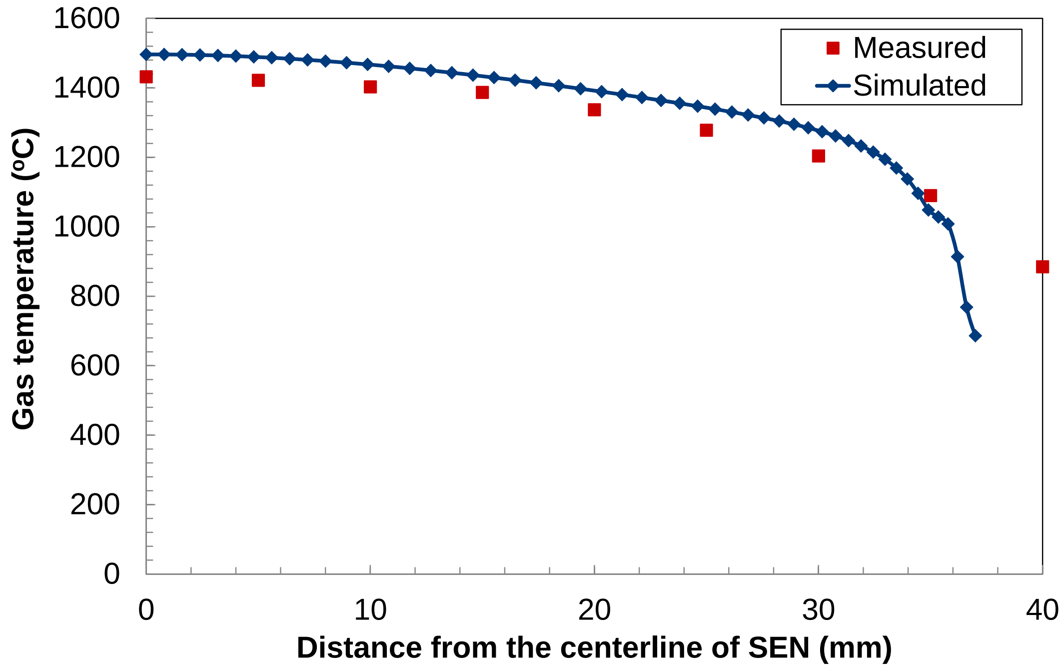
Pressure Outlet

Gauge Pressure (Pa)		0
Turbulent Kinetic Energy (m^2/s^2)		0
Turbulent Dissipation Rate (m^2/s^3)		0
Backflow Temperature (℃)		26.85
Mean Mixture Fractio Air (oxidant)		0
Mixture Fraction Variance		0
Radiation	Black body temp. (℃)	26.85
	Internal Emissivity	10^{-11}

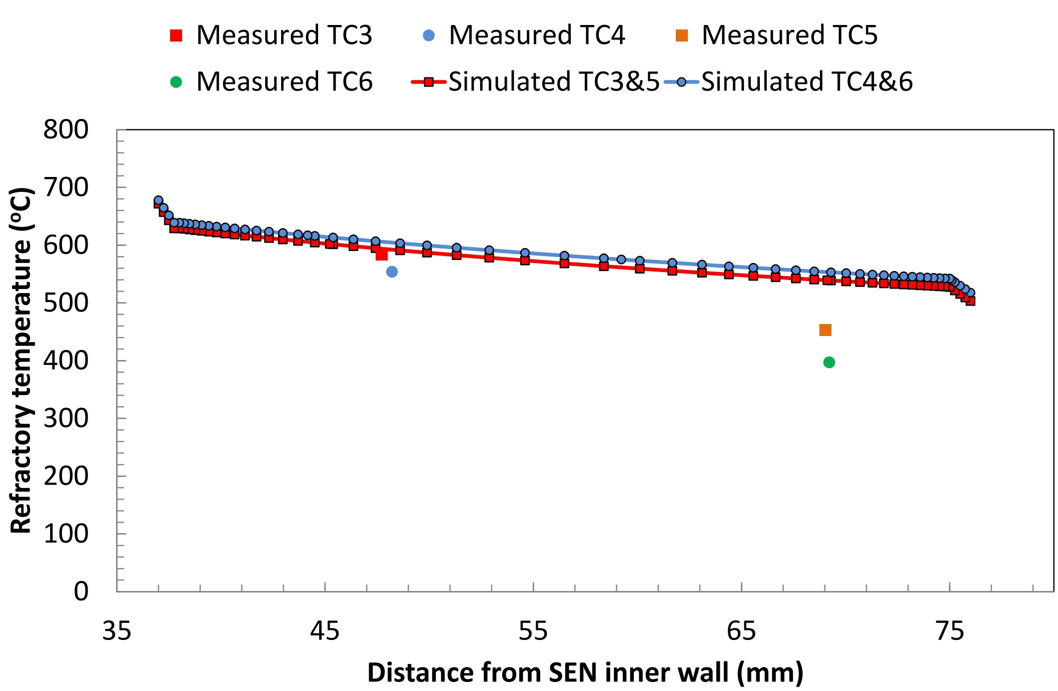
Initialization conditions

Non-premixed model Initialization	**Value**
Initialization Method	Standard Initialization
Compute From	Mixture inlet
Reference Frame	Relative to Cell Zone
Temperature (℃)	3104.67
Axial Velocity (m/s)	26.48
Turbulent Kinetic Energy (m^2/s^2)	0
Turbulent Dissipation Rate (m^2/s^3)	0
Mixture Fraction Variance	0
Mean Mixture fraction	1

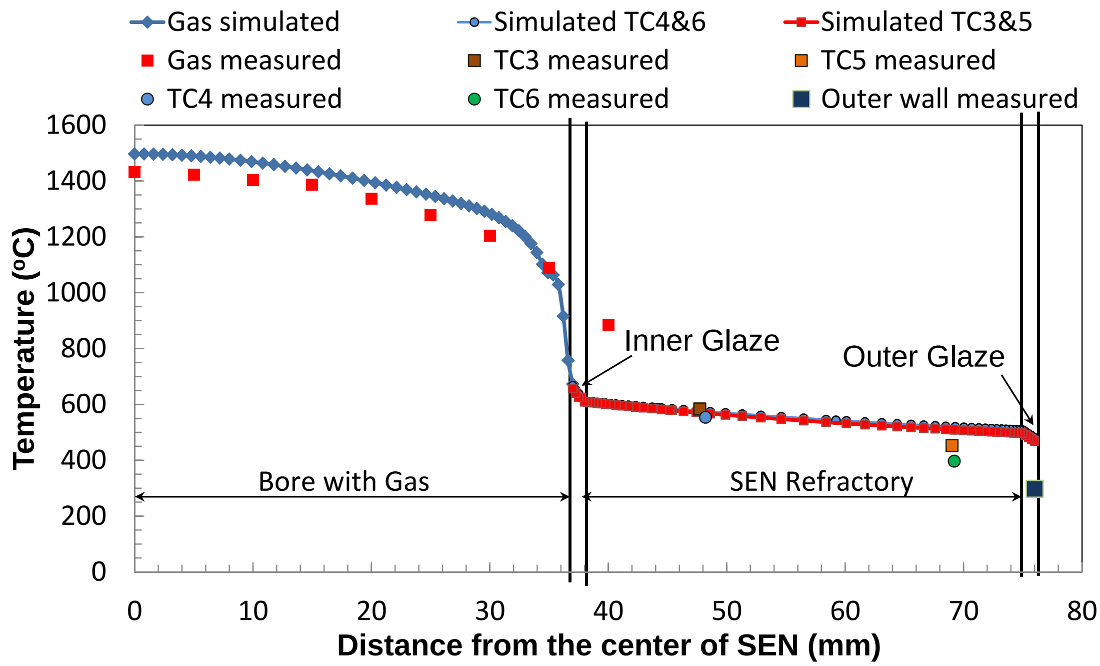
Gas Temperature Validation (measured by Thermocouple 1)



Solid Temperature Validation (measured by Thermocouple 3-6)



Model validation: Temperature



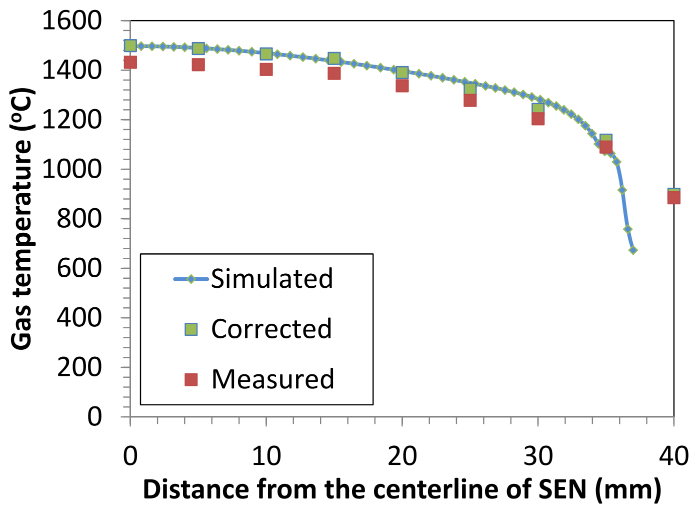
Adjust Gas Temperature Measurement

The gas temperature measurements must be corrected for the errors due to radiation, convection, and wire conduction from the thermocouple junction. Conduction is neglected for wires over 1mm long[10]. The radiation from the environment to the junction has been neglected.

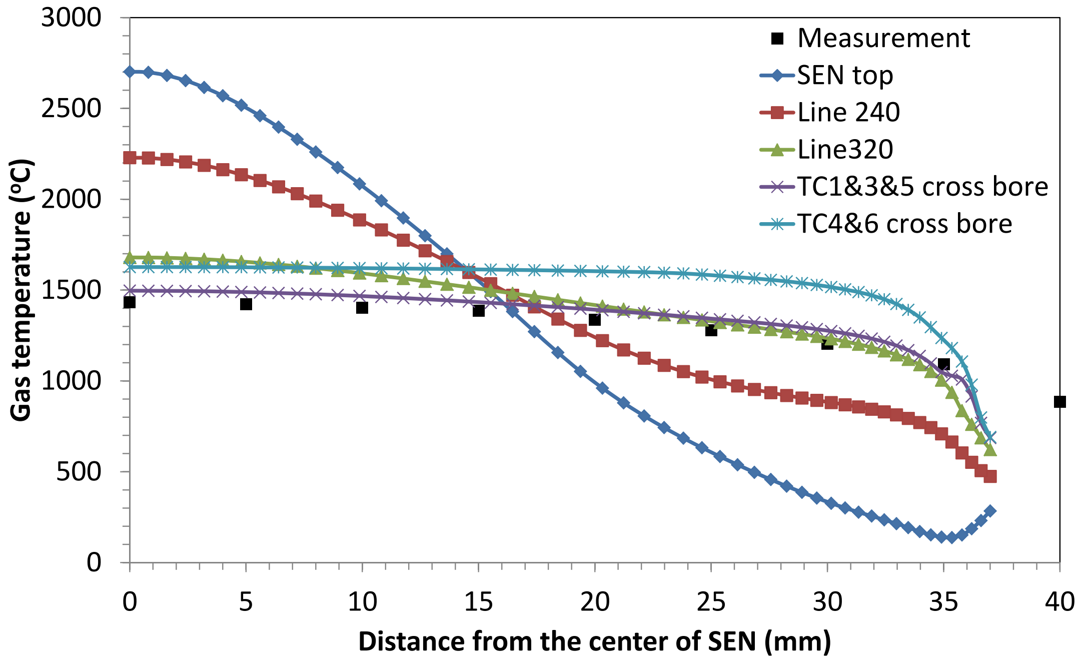
Simplify into:

$$t_j = t_{T/C} + \sigma \varepsilon_{T/C} {t_{T/C}}^4 / h$$

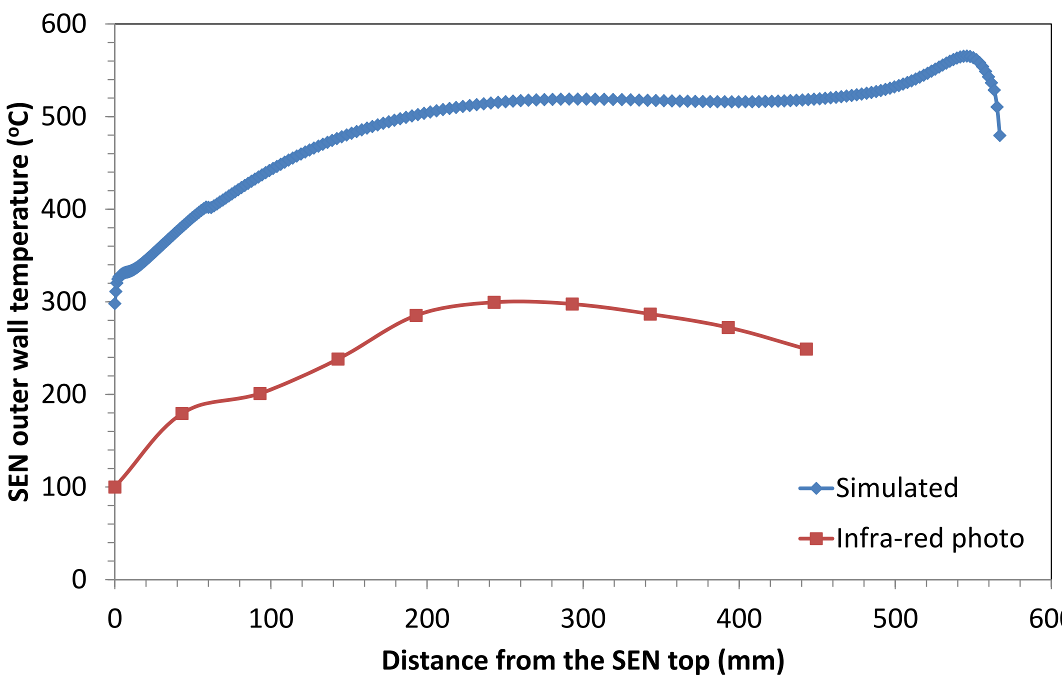
Where t_j is the corrected temperature; $t_{T/C}$ is measured temperature by the thermocouple; σ is Stefan-Boltzmann constant; $\varepsilon_{T/C}$ is probe emissivity (0.14 was recommended for uncoated platinum Type B thermocouple); h is convection coefficient for gas flowing over probe (1000 W/m²K is used).



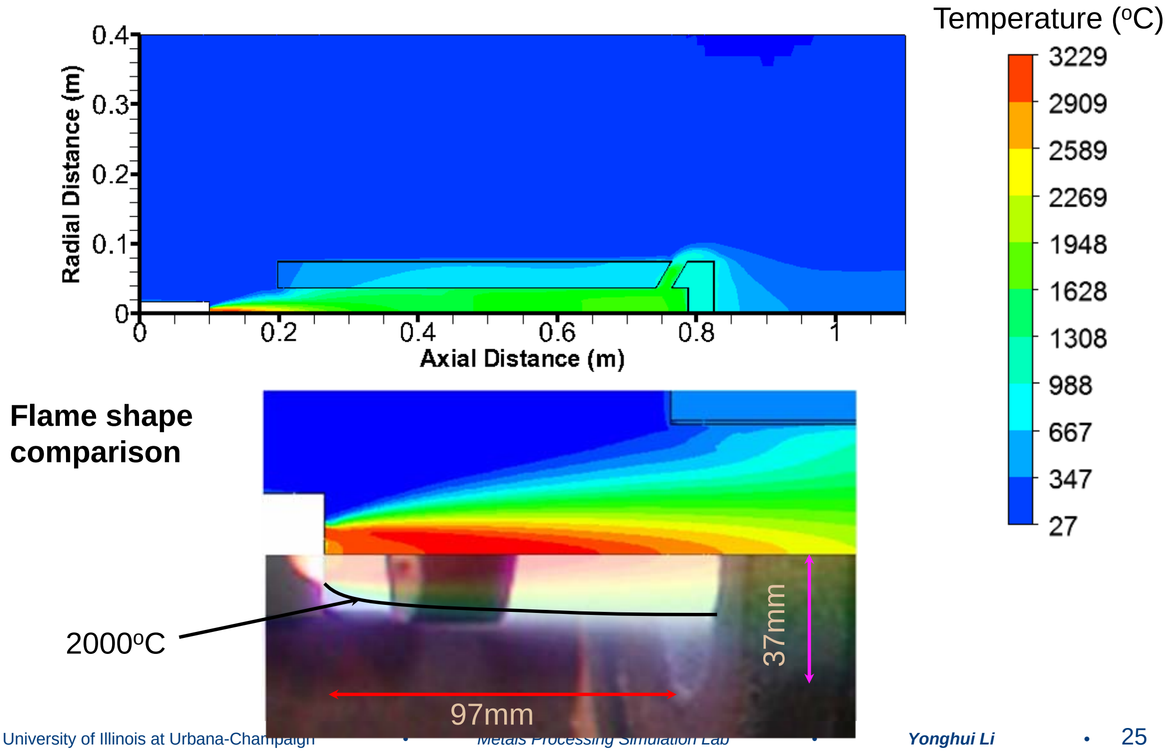
Gas Temperature profiles across SEN at different axial distances down SEN



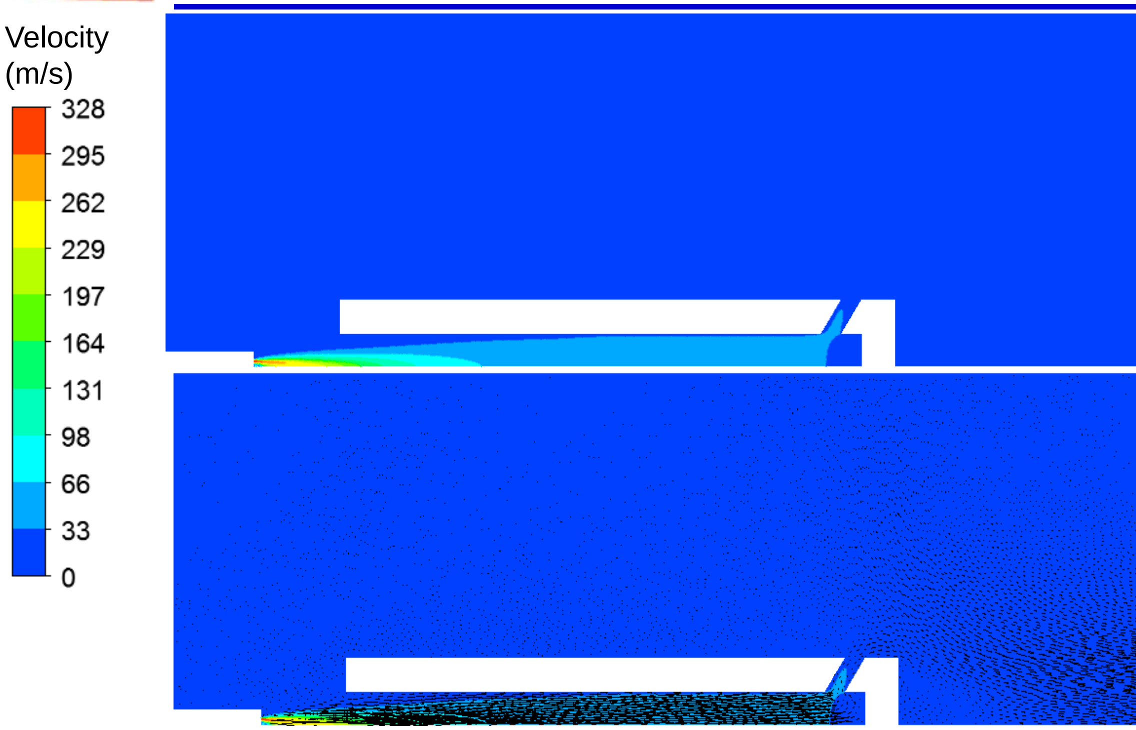
SEN Outer Wall Temperature



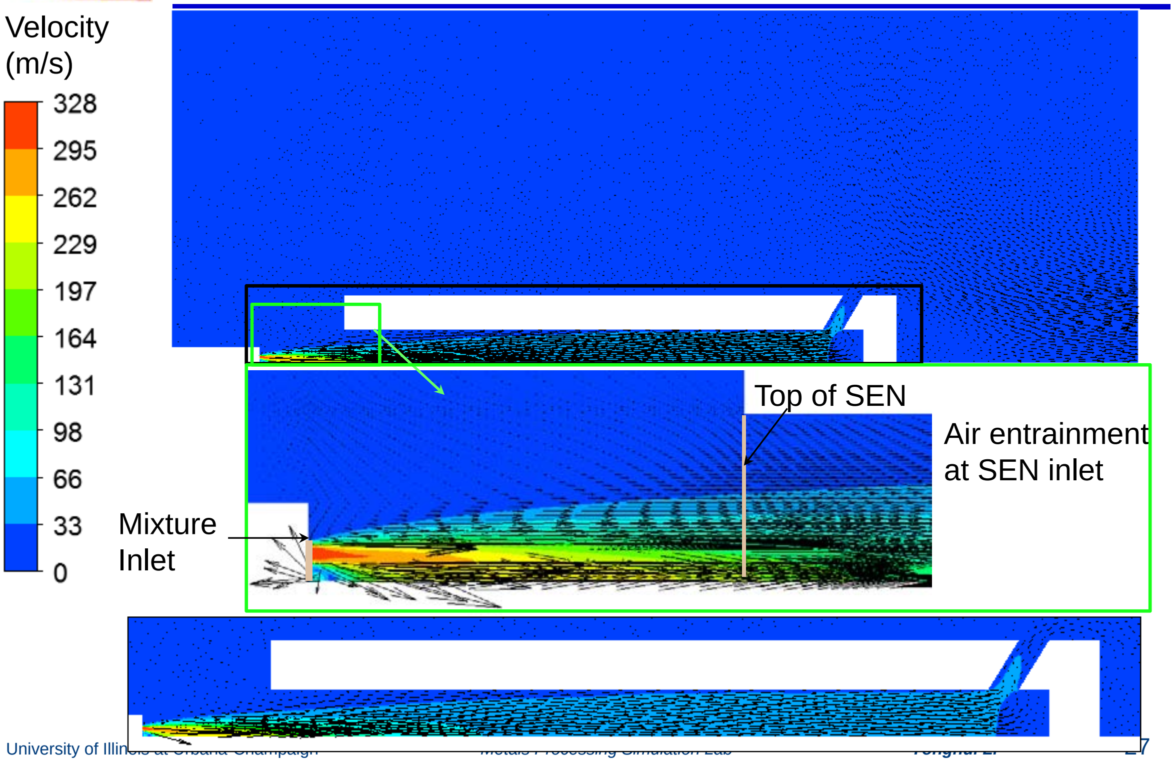
Temperature Contour Validate the Flame Shape



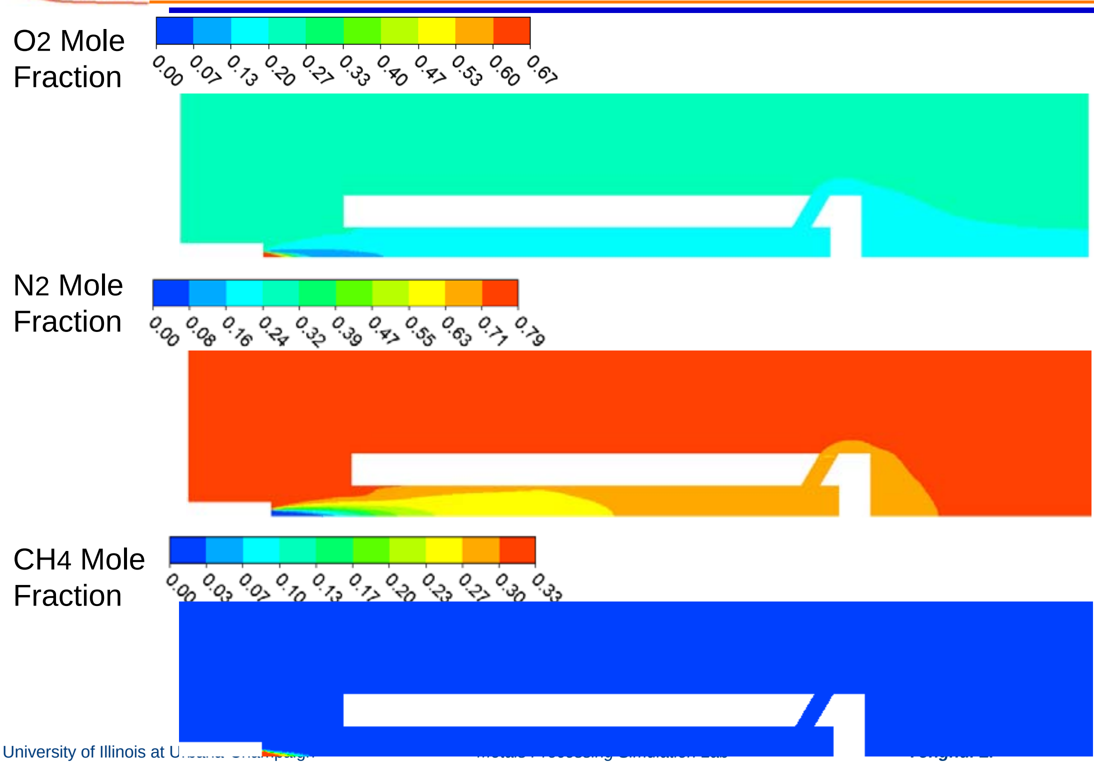
Velocity Contour and Vector



Zoom in Velocity Vector

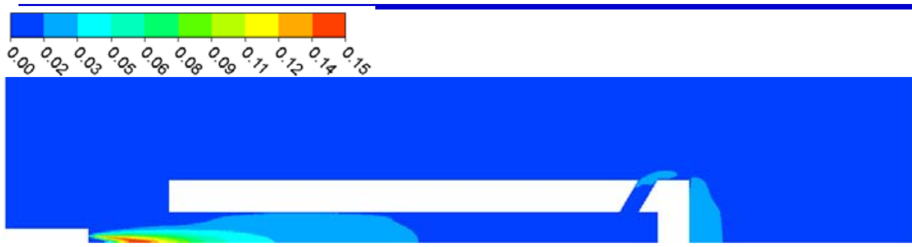


Mole fraction of Reactants

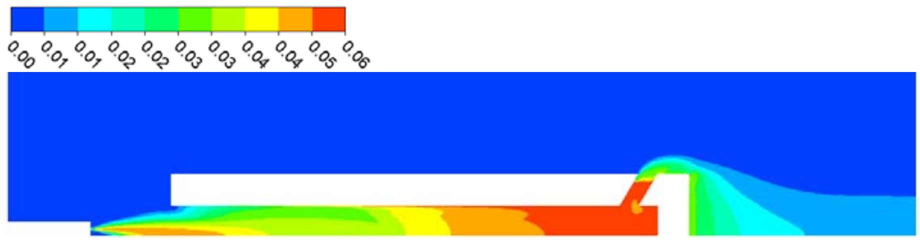


Mole fraction of Main Productions

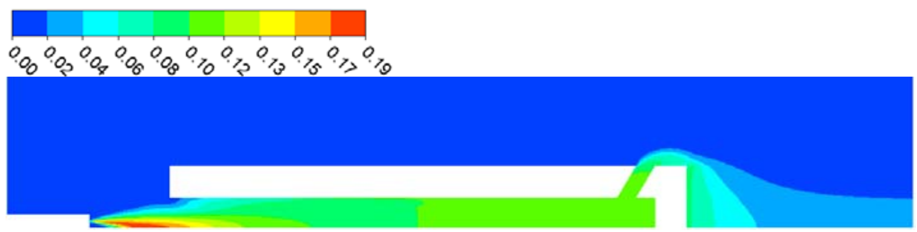
CO Mole Fraction



CO2 Mole Fraction



H2O Mole Fraction



Compositions down Nozzle Centerline

Mole fraction of compositions down the nozzle centerline

	Top of SEN	TC1 Cross Bore	TC4 Cross Bore	Center of Port Inside	Center of Port Outside
Temperature	$2975^{o}C$	$1770^{o}C$	$1928^{o}C$	$1914^{o}C$	$1181^{o}C$
N2	26.97%	60.60%	63.47%	64.90%	63.41%
O2	10.80%	16.40%	16.50%	16.90%	17.10%
H2O	17.30%	9.36%	9.88%	10.60%	8.27%
CO	10.53%	2.48%	1.17%	0.33%	2.02%
CO2	4.82%	3.53%	4.46%	5.21%	3.14%
OH	8.72%	1.55%	1.28%	0.60%	1.07%
O	7.68%	3.00%	1.48%	0.46%	2.52%
H	7.62%	2.08%	0.68%	0.15%	1.75%
H2	5.24%	0.85%	0.40%	0.12%	0.64%
Sum	99.68%	99.85%	99.32%	99.27%	99.92%
Minor	NO, CH3, N, HCO, HO2, CH2O, CH2OH, CH2, C, CH2<S>, CH, NH, NO2, H2O2, HCCO, HNO, N2O, CH3O, CH3OH, HCN, CH4				

30 species total.

Oxygen Source Fraction and Air Entrainment

- Definitions[11]
  - **Oxygen source fraction** is the ratio of oxygen amount relative to stoichiometric reaction oxygen requirement. The oxygen source fraction of stoichiometric combustion is 100%.
  - **Air Entrainment** is the ratio of current amount of air relative to the amount of air needed for stoichiometric combustion.
- Equations[11]
  - $Oxygen\ Source\ Fraction\ in\ mole\ flow\ rate = \frac{\dot{n}_{O_2}}{2\dot{n}_{CH_4}}$
  - $Air\ Entrainment\ in\ air\ mass\ flow\ rate = \frac{\dot{m}_{air} * \frac{79}{21}}{\left(\frac{79}{21}+1\right) * MW_{air} * 2 * \frac{79}{21} * \dot{n}_{CH_4}}$
- Input of Oxygen Source Fraction for FLUENT and Output Air Entrainment

Oxygen Source Fraction is 100%.

Air Entrainment Flow Rate (kg/s)	
Mixture Inlet	4.709×10^{-3}
SEN Upper Inlet	29.376×10^{-3}
Entrained Air	24.667×10^{-3}
Air Entrainment	151.955%

Two methods[11] to obtain air entrainment from FLUENT

- Method 1
  - Increment of the mass flow rate is caused by entrained air.

Total Mass Flow Rate (kg/s)	
Mixture Inlet	4.709×10^{-3}
SEN Upper Inlet	29.376×10^{-3}
Entrained Air	24.667×10^{-3}
Air Entrainment	**152.0%**

$$Air\ Entrainment = 30.15\% * \frac{\dot{m}_{air} * T_{CH_4}}{P_{CH_4} * \dot{V}_{CH_4}}$$

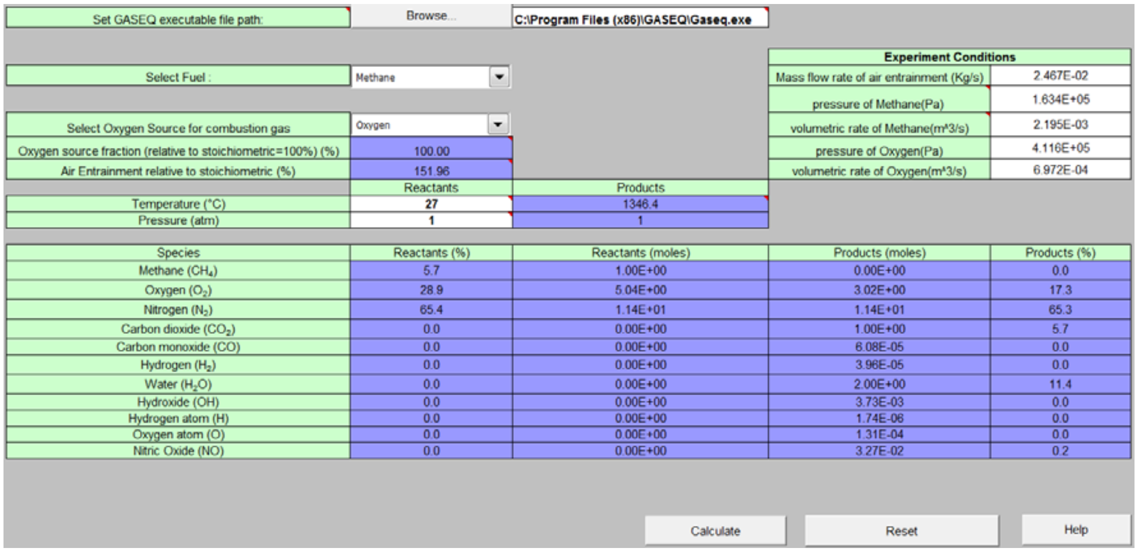
The increase of total mass flow rate is caused by entrained air.

- Method 2
  - Based on N_2 mass balance (barely N_2 participates reaction)

Specific Mass Flow Rate (kg/s)	
N_2 SEN Upper Inlet	4.709×10^{-3}
CH_4 Mixture Inlet	29.376×10^{-3}
Air Entrainment	**152.2%**

$$Air\ Entrainment = \frac{\dot{m}_{N_2} MW_{CH_4}}{2 * \frac{79}{21} * \dot{m}_{CH_4} MW_{N_2}}$$

Flame Temperature VBA Model[12] Predicted by Gaseq[13]



Set GASEQ executable file path:	Browse...	C:\Program Files (x86)\GASEQ\Gaseq.exe
Select Fuel :	Methane	
Select Oxygen Source for combustion gas	Oxygen	
Oxygen source fraction (relative to stoichiometric=100%) (%)	100.00	
Air Entrainment relative to stoichiometric (%)	151.96	
	Reactants	Products
Temperature (°C)	27	1346.4
Pressure (atm)	1	1

Experiment Conditions	
Mass flow rate of air entrainment (Kg/s)	2.467E-02
pressure of Methane(Pa)	1.634E+05
volumetric rate of Methane(m^3/s)	2.195E-03
pressure of Oxygen(Pa)	4.116E+05
volumetric rate of Oxygen(m^3/s)	6.972E-04

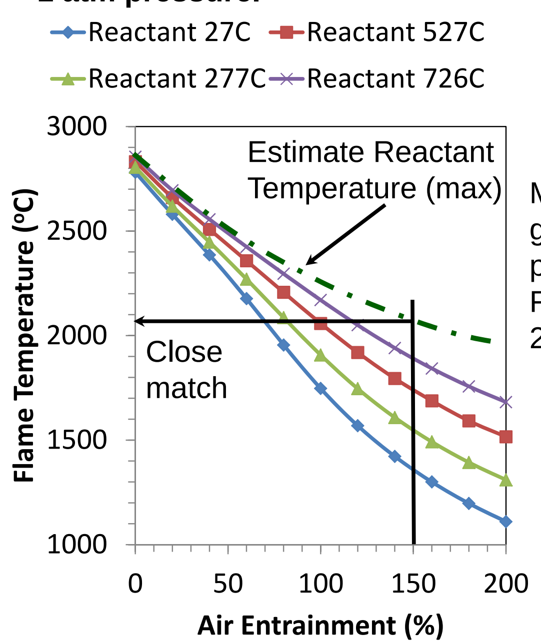
Species	Reactants (%)	Reactants (moles)	Products (moles)	Products (%)
Methane (CH_4)	5.7	1.00E+00	0.00E+00	0.0
Oxygen (O_2)	28.9	5.04E+00	3.02E+00	17.3
Nitrogen (N_2)	65.4	1.14E+01	1.14E+01	65.3
Carbon dioxide (CO_2)	0.0	0.00E+00	1.00E+00	5.7
Carbon monoxide (CO)	0.0	0.00E+00	6.08E-05	0.0
Hydrogen (H_2)	0.0	0.00E+00	3.96E-05	0.0
Water (H_2O)	0.0	0.00E+00	2.00E+00	11.4
Hydroxide (OH)	0.0	0.00E+00	3.73E-03	0.0
Hydrogen atom (H)	0.0	0.00E+00	1.74E-06	0.0
Oxygen atom (O)	0.0	0.00E+00	1.31E-04	0.0
Nitric Oxide (NO)	0.0	0.00E+00	3.27E-02	0.2

Calculate | Reset | Help

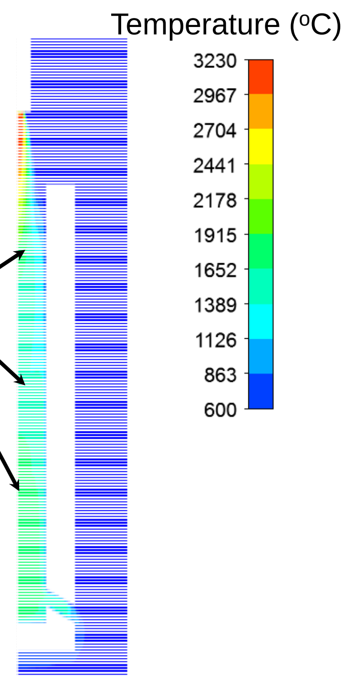
- In the condition of 27 °C and 1 atm, the flame temperature is 1346°C.
- The maximum reactants temperature is 726°C (999K). With 1 atm, the flame temperature is 1881°C.
- Gaseq predicts products average temperature for equilibrium adiabatic conditions.

Flame Temperatures Predicted by Gaseq

100% oxygen source mole fraction
1 atm pressure.

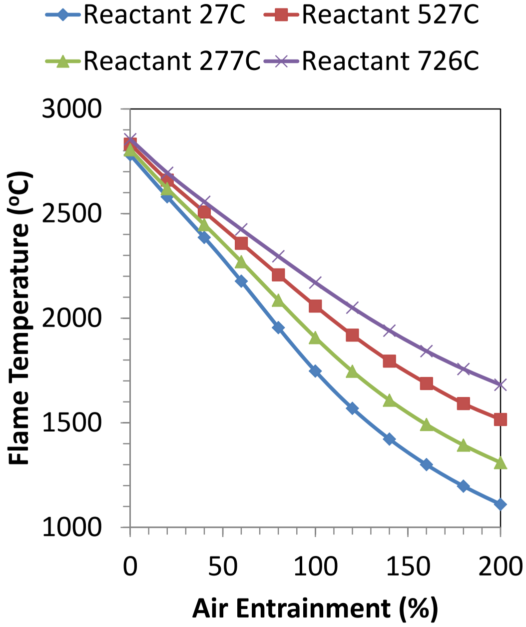


Most SEN inner gas temperature predicted by FLUENT is around 2000°C.

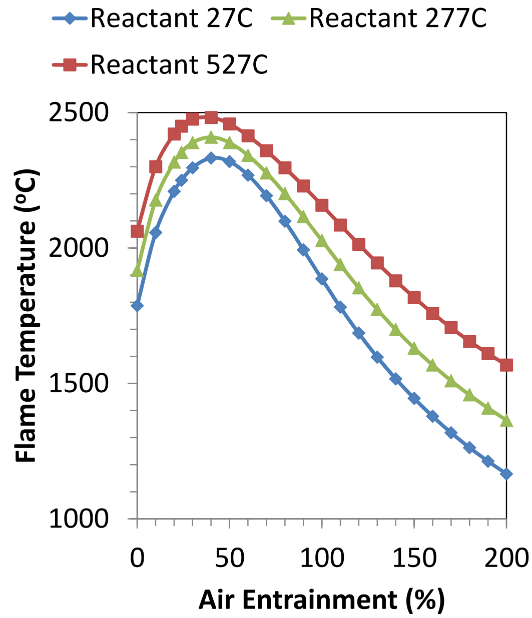


Flame Temperatures Predicted by Gaseq

100% oxygen source mole fraction
1 atm pressure.



40% oxygen source mole fraction
1 atm pressure.



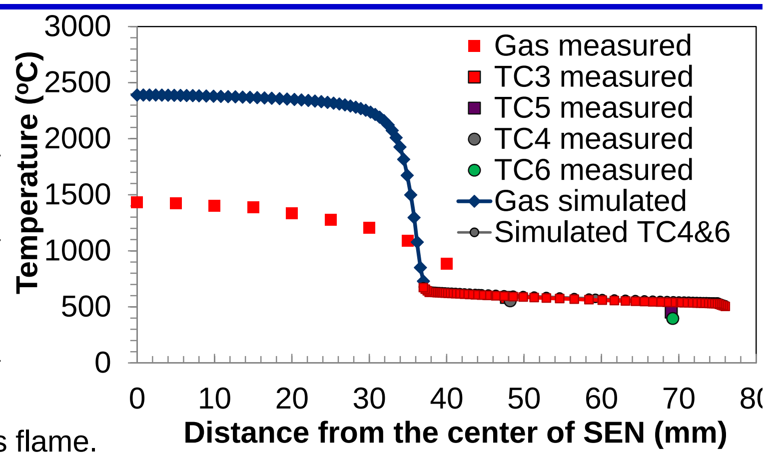
Results assuming equilibrium combustion: too hot

Different Model Settings:

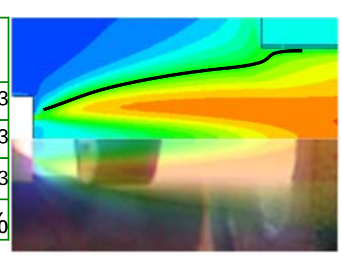
All identical except:

State Relation	Equilibrium
Fuel Stream Rich Flamability limit	0.8
Boundary, fuel, mixture inlet temperatures	526.85ºC
Emissivity	0.7*

* 0.7 high emissivity for luminous flame.



Total Mass Flow Rate (kg/s)	
Mixture Inlet	4.709×10^{-3}
SEN Upper Inlet	11.266×10^{-3}
Entrained Air	6.557×10^{-3}
Air Entrainment	40.0%



Equilibrium assumption causes too much earlyl expansion of the flame, which prevents air entrainment. **Less air entrainment** increases gas temperature in nozzle.

Conclusions

- 2D steady-state axisymmetric non-equilibrium combustion model is developed using FLUENT, with Non-premixed Species Flamelet Model and 88843 quadrilateral cell mesh.
- The experiment volume flow rate is corrected based on measured pressure, due to white/blue flame observation (very near stoichiometric).
- The shape of the flame down rosebud matches well with experimental photo.
- Model matches with measured temperatures of TC1 within 67^{o}C error. After correcting for convection and radiation heat loss, the model matches mostly within 8^{o}C error and 39^{o}C near boundary.
- The predicted SEN wall temperatures match experiments in the acceptable domain.
- Flame temperature model with Gaseq can predict the flame temperature by given measurement and air entrainment.

Future Work

- Transient heat flow in nozzle wall

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- Rob Nonnington from Magnesita Refractories

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