High-Pressure Turbulent Flame Speeds and Chemical Kinetics of Syngas Blends With and Without Impurities

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Project Overview

Project Began in October, 2013

Project Highlights:

1. Duration: **Oct. 1, 2013 – Sept. 30, 2017**
2. DOE NETL Award **DE-FE0011778**
3. Budget: $498,382 DOE + $124,595 Cost Share
4. Principal Investigator: Dr. Eric L. Petersen

Project Overview

This Project Addressed Several Problems for HHC Fuels

1. Improve **NOx kinetics** for High-Hydrogen Fuels at Engine Conditions

2. Effect of **Contaminant Species** on Ignition and Flame Speed

3. Impact of **Diluents** on Ignition Kinetics and Flame Speeds

4. Data on **Turbulent Flame Speeds** at Engine Pressures

Project Overview

There Were Five Main Work Tasks for the Project

Work Tasks:

Task 1 – Project Management and Program Planning

Task 2 – Turbulent Flame Speed Measurements at Atmospheric Pressure

Task 3 – Experiments and Kinetics of Syngas Blends with Impurities

Task 4 – Design and Construction of a High-Pressure Turbulent Flame Speed Facility

Task 5 – High-Pressure Turbulent Flame Speed Measurements

Project Publications

6 Journal Publications from Project to Date

Journal Publications

1) O. Mathieu, C. Mulvihill, and E. L. Petersen, "Shock-Tube Water Time-Histories and Ignition Delay Time Measurements for H_2S Near Atmospheric Pressure," *Proceedings of the Combustion Institute*, Vol. 36, 2017, pp. 4019-4027.

2) O. Mathieu, B. Giri, A. R. Agard, T. N. Adams, J. D. Mertens, and E. L. Petersen, "Nitromethane Ignition Behind Reflected Shock Waves: Experimental and Numerical Study," *Fuel*, Vol. 182, 2016, pp. 597-612.

3) N. Donohoe, K. A. Heufer, C. J. Aul, E. L. Petersen, G. Bourque, R. Gordon, and H. J. Curran, "Influence of Steam Dilution on the Ignition of Hydrogen, Syngas and Natural Gas Blends at Elevated Pressures," *Combustion and Flame*, Vol. 162, 2015, pp. 1126-1135.

4) O. Mathieu and E. L. Petersen, "Experimental and Modeling Study on the High-Temperature Oxidation of Ammonia and Related NOx Chemistry," *Combustion and Flame*, Vol. 162, 2015, pp. 554-570.

5) S. Ravi, T. G. Sikes, A. Morones, C. L. Keesee, and E. L. Petersen, "Comparative Study on the Laminar Flame Speed Enhancement of Methane with Ethane and Ethylene Addition," *Proceedings of the Combustion Institute*, Vol. 35, Issue 1, 2015, pp. 679-686.

6) O. Mathieu, J. W. Hargis, A. Camou, C. Mulvihill, and E. L. Petersen, "Ignition Delay Time Measurements Behind Reflected Shock Waves for a Representative Coal-Derived Syngas With and Without NH_3 and H_2S Impurities," *Proceedings of the Combustion Institute*, Vol. 35, Issue 3, 2015, pp. 3143-3150.

Conference Publications

11 Conference Papers to Date

In Preparation

2 Journal Papers

Task 4 – Design and Construction of a Turbulent Flame Speed Facility

Task 4 – New Facility

New Facility Designed and Built at TAMU

1. Detailed Design and Structural Analysis

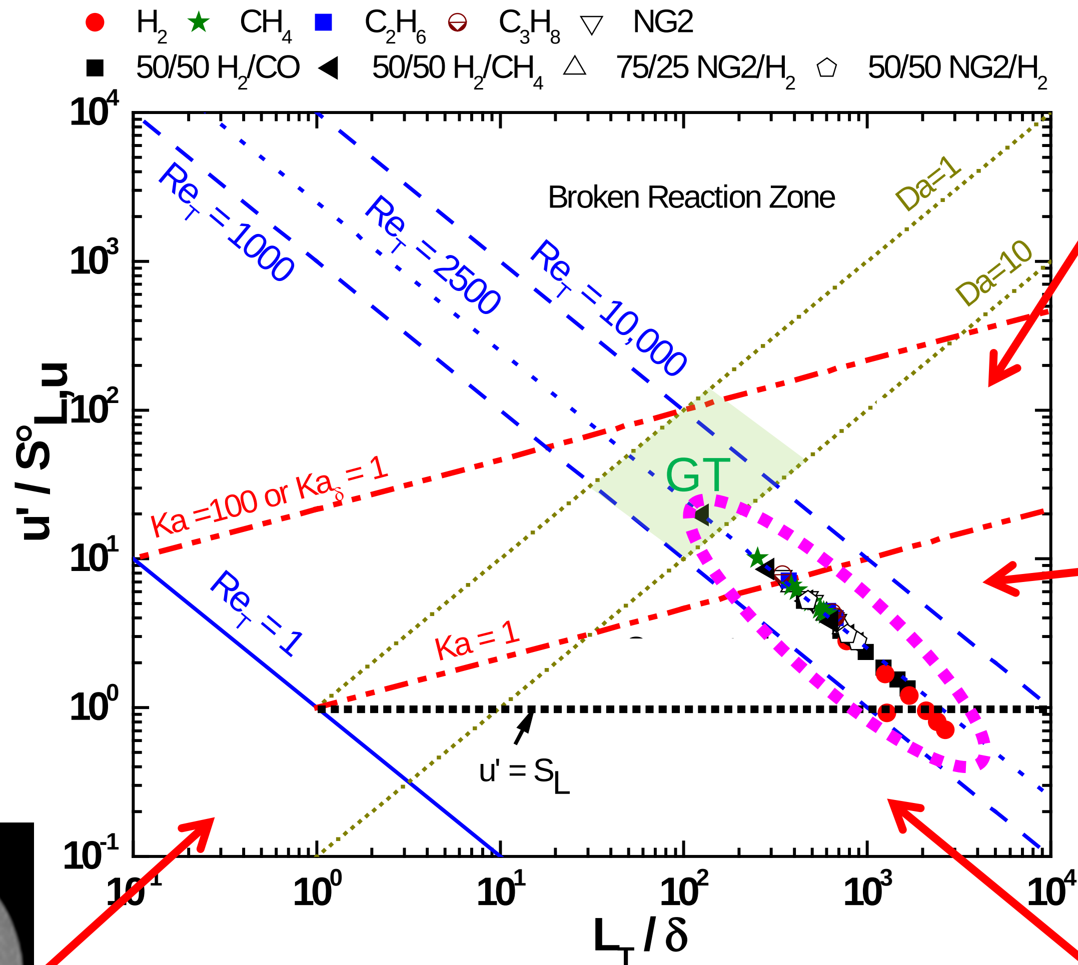
2. Fabrication of Vessel Components

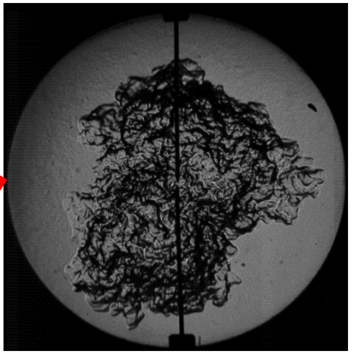
3. Installation of Vessel

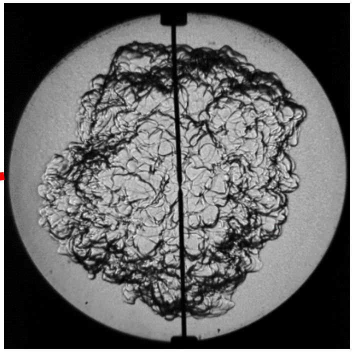
4. Characterization of Flow Conditions

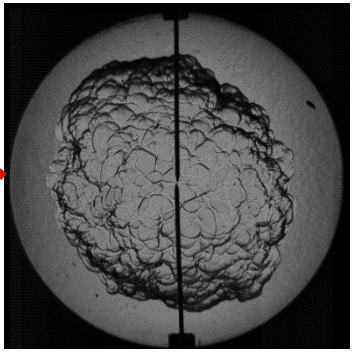
Combustion regimes

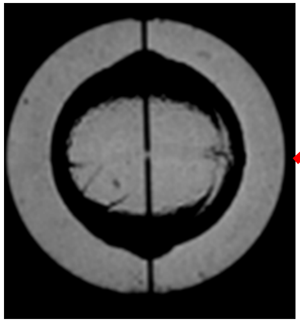
Recent data cover a wide range of flamelet regions











(Ravi, Petersen 2014)

Opportunities and objectives

*Targets for **New Turbulent Flame Bomb***

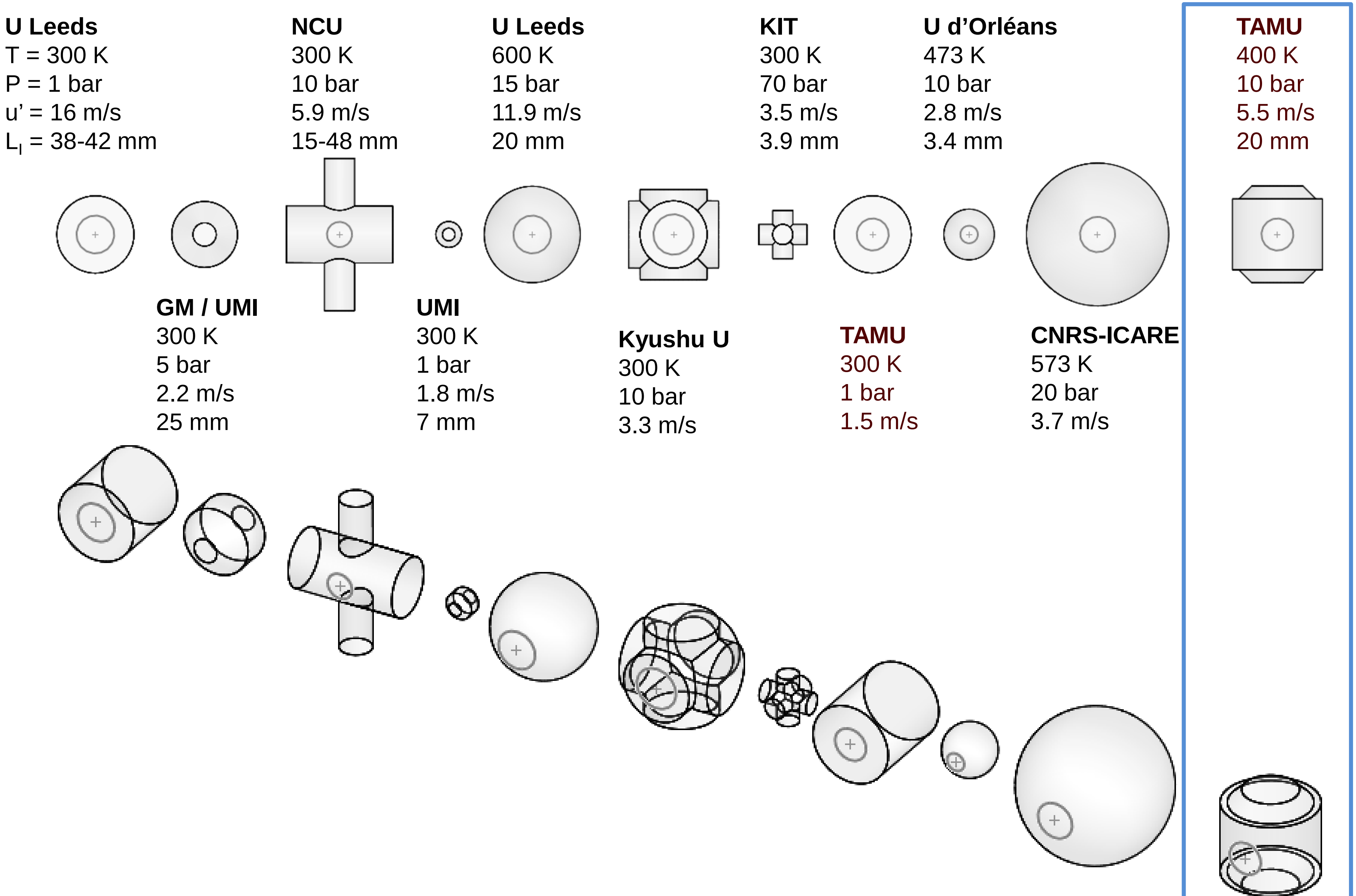
1. High-pressure / temperature data are limited

2. Refined diagnostics for local stretch are needed

3. Higher levels of well-characterized turbulence are desired

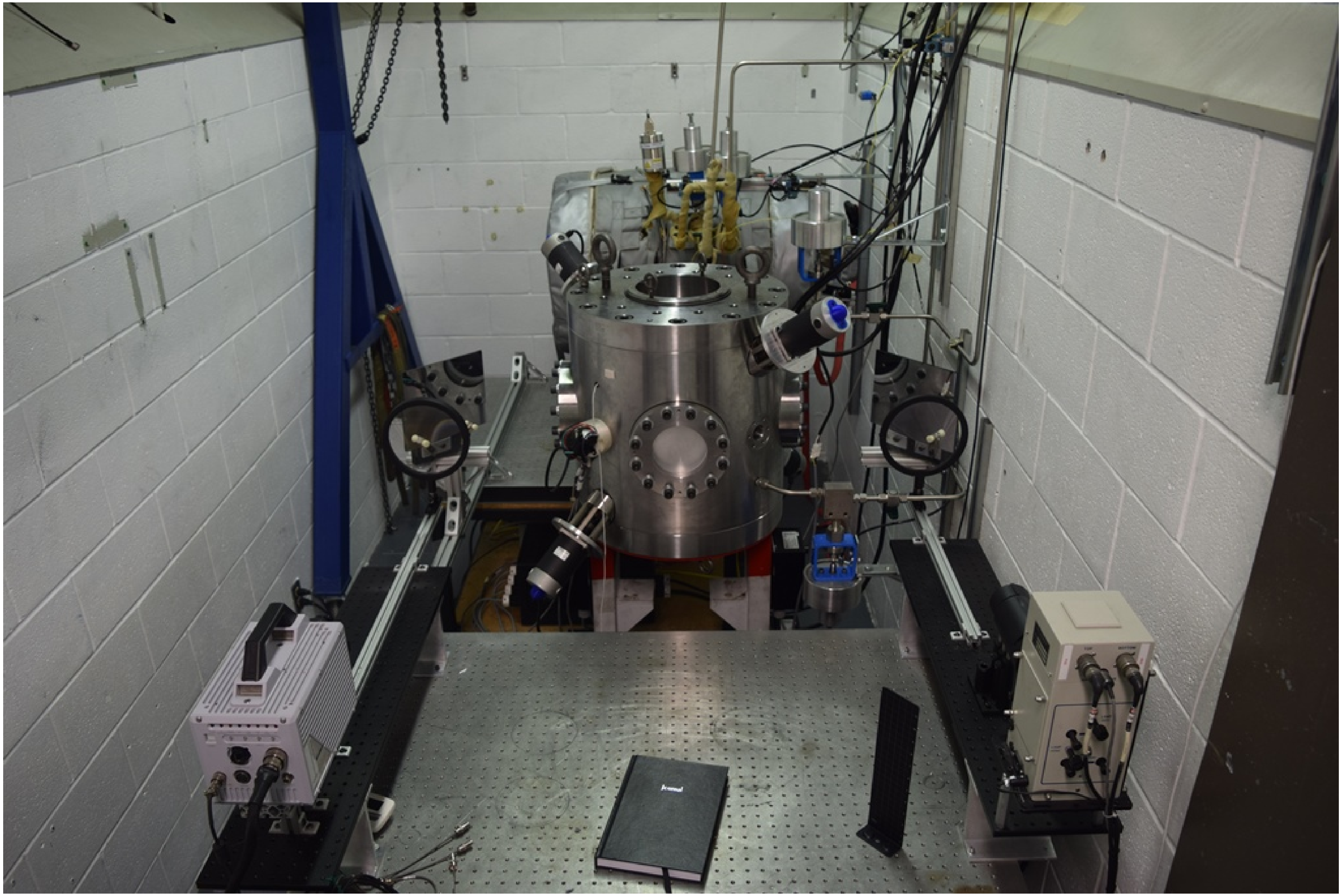
Facility survey

Few bombs with high pressure, temperature and u' capabilities



New turbulent flame speed bomb

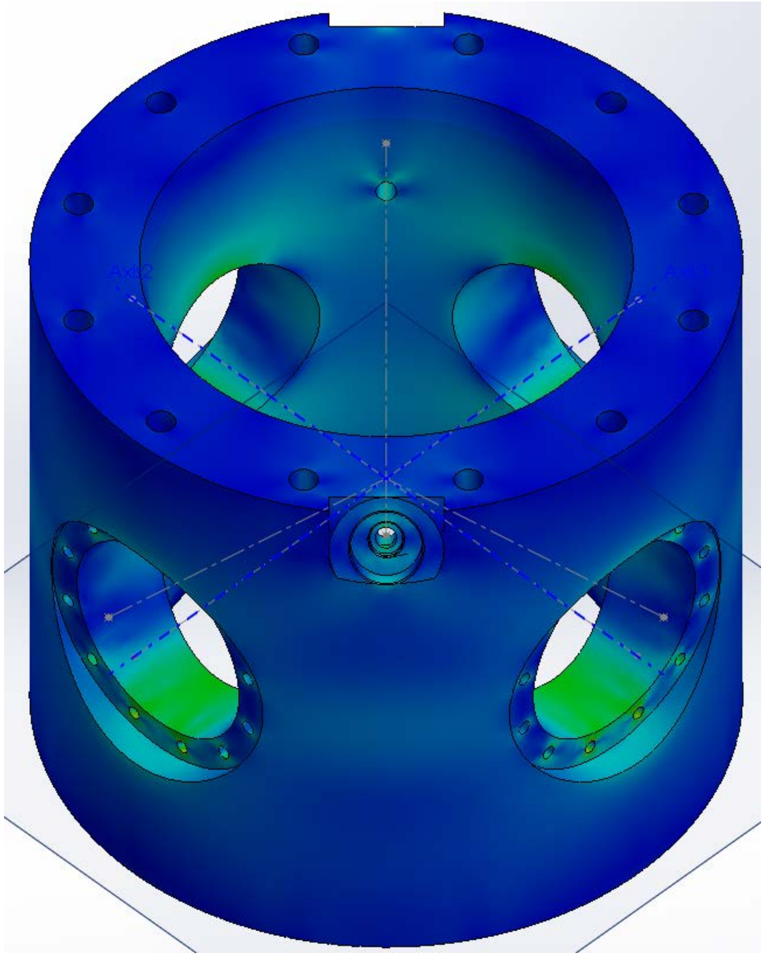
New layout optimized available space and facilities



Mechanical Design

The vessel

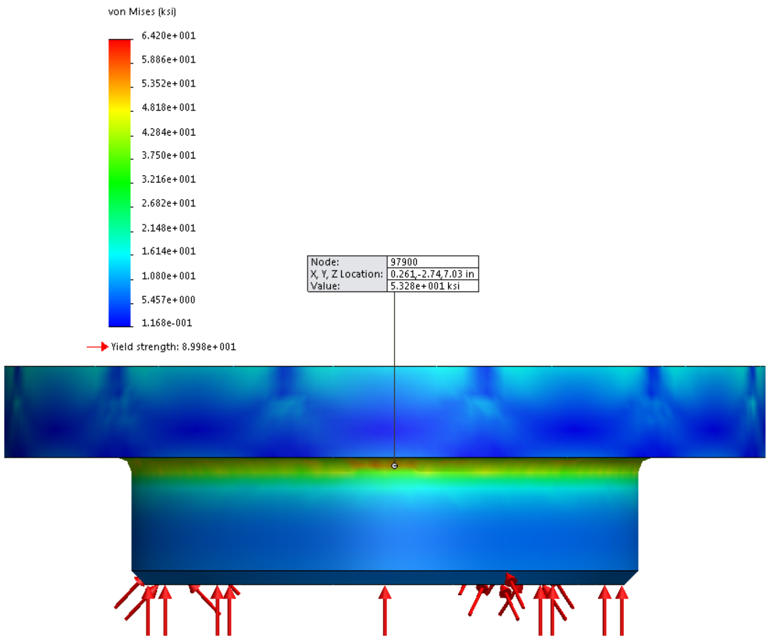
Familiar design with improvements



Built forged SS seamless rings

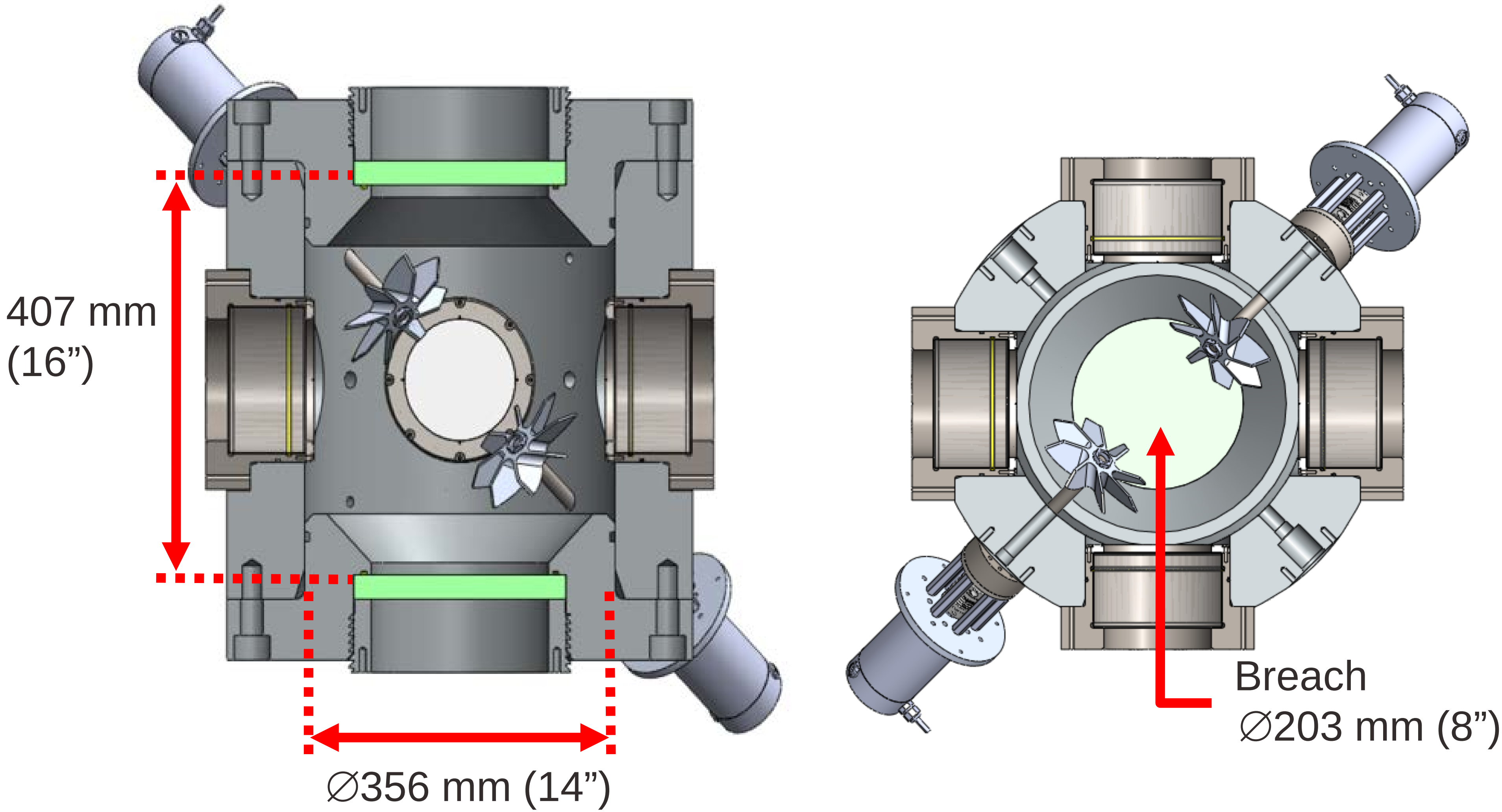
Max. pressure 1500 psi

Max. temp 400 K (o-ring limited)



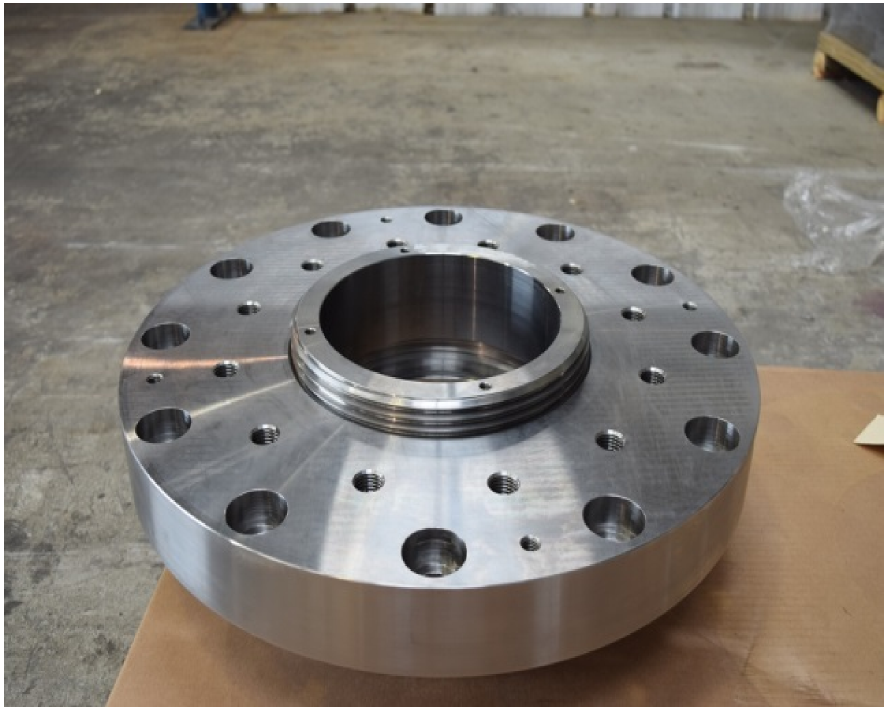
Vessel dimensions

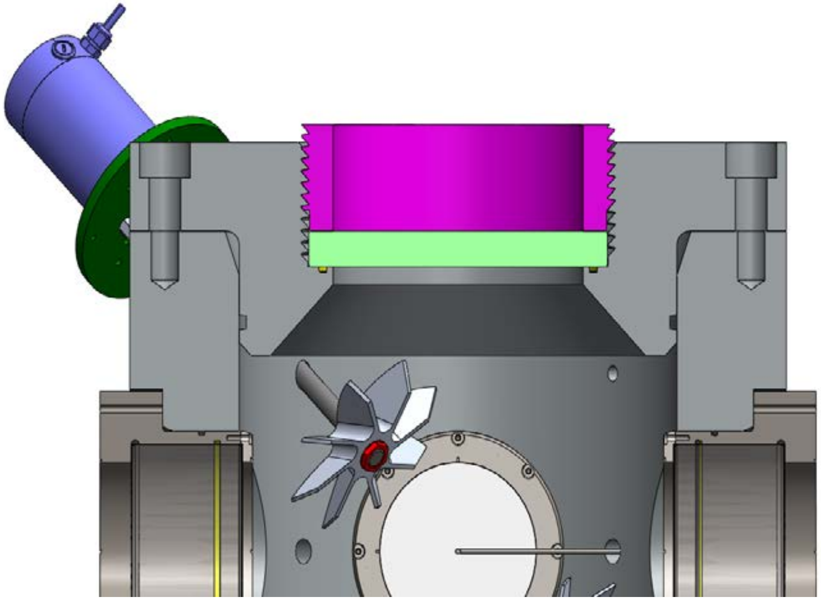
Window aperture-to-ID ratio = 36%



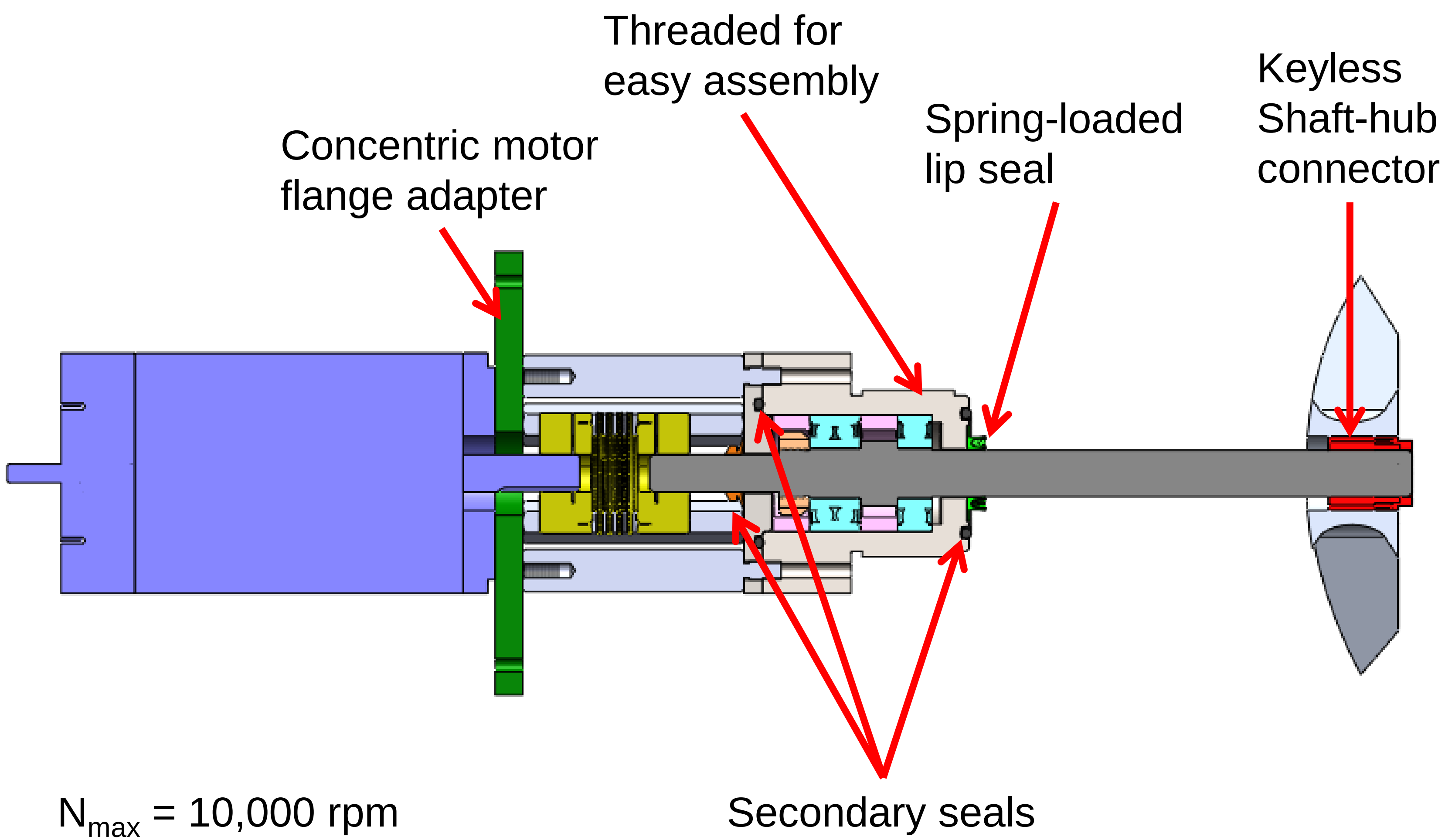
Breech

Strong, versatile, and generous access





Stirring assembly

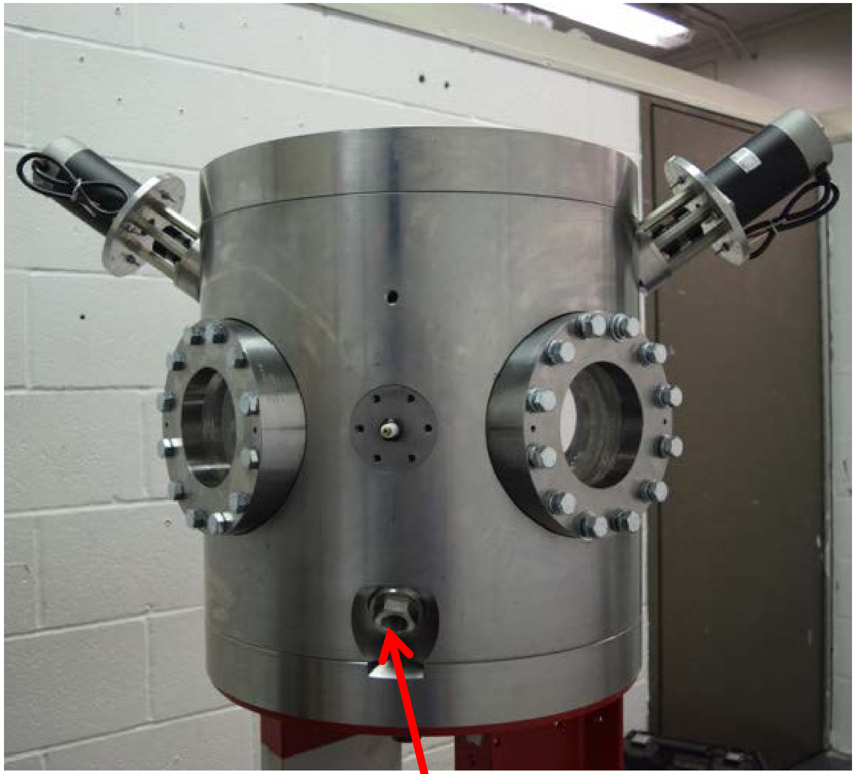


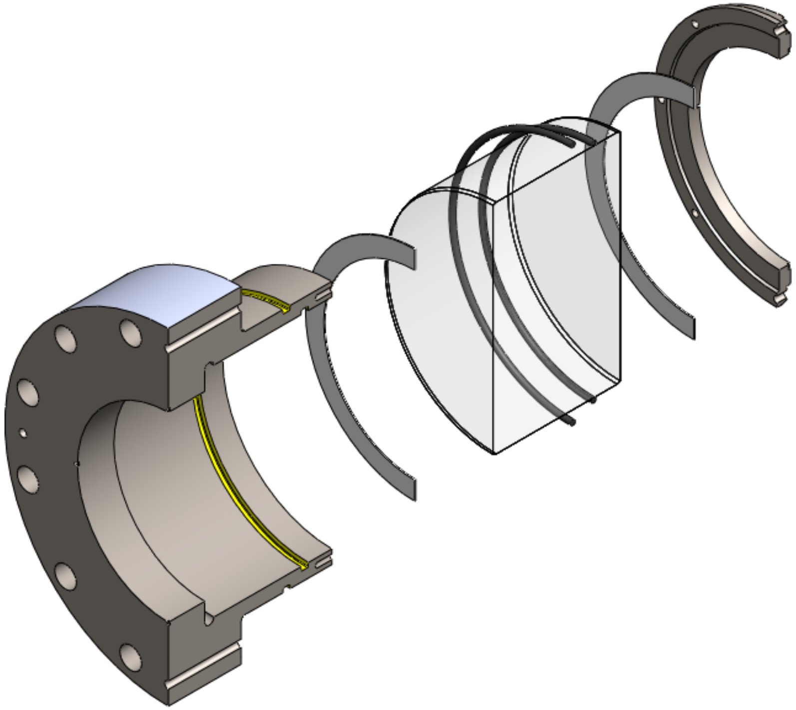
N_{max} = 10,000 rpm
P_0 = 100 mTorr achieved

Windows

Two orthogonal lines of sight. Aperture ⌀ = 5 in

Designed for 3000 psi





Low-stress window mount.
Easy assembly

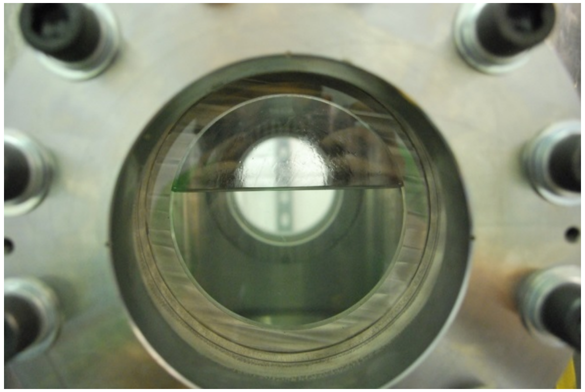
Stirring port plug for quiescent experiments

Fasteners

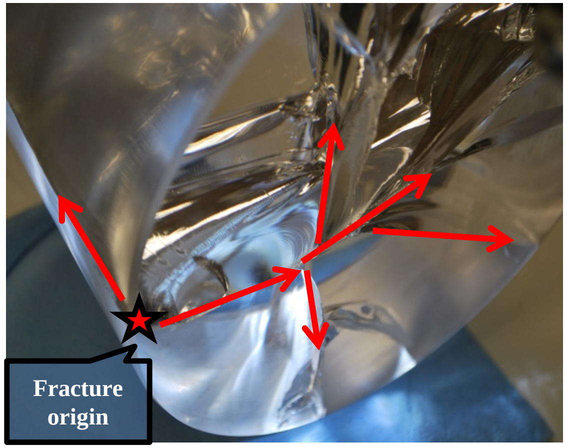
Application	Thread	Number of fasteners	Q, corrected engagement length, in	Fastener strength, ksi	Pressure, psi	Total load, lb	Load per fastener, lb	Fastener, load capacity, lb	Safety factor
Window clamp	8-32 UNC 2A	8	0.137	180	15	416	52	2,522	48.5
Housing cover	1/4-20 UNC 2A	12	0.182	170	3,000	9,425	785	5,410	6.9
Side port	5/16-18 UNC 2A	6	0.238	170	3,000	4,455	742	8,913	12.0
Window cell	9/16-12 UNC 2A	12	0.442	170	3,000	107,355	8,946	30,931	3.5
Spark plug	1/2-14 NPT	1		110	3,000	1,663	1,663	51,277	30.8
Expansion joint	7/8-9 UNC 2A	12	0.705	170	3,000	235,619	19,635	78,495	4.0
End cap	1-8 UNC 2A	12	0.802	170	3,000	461,814	38,485	102,977	2.7
Bearing housing	2 1/4 -10 UNS 2A	1	1.853	110	3,000	2,356	2,356	400,311	169.9
Retaining ring	10-3 BUTT 3A	1	0.1439	63.5†	3,000	235,619	235,619	3,928,462	16.7

Hydrostatic test

Hydrostatic test successful and resulted in improved window design

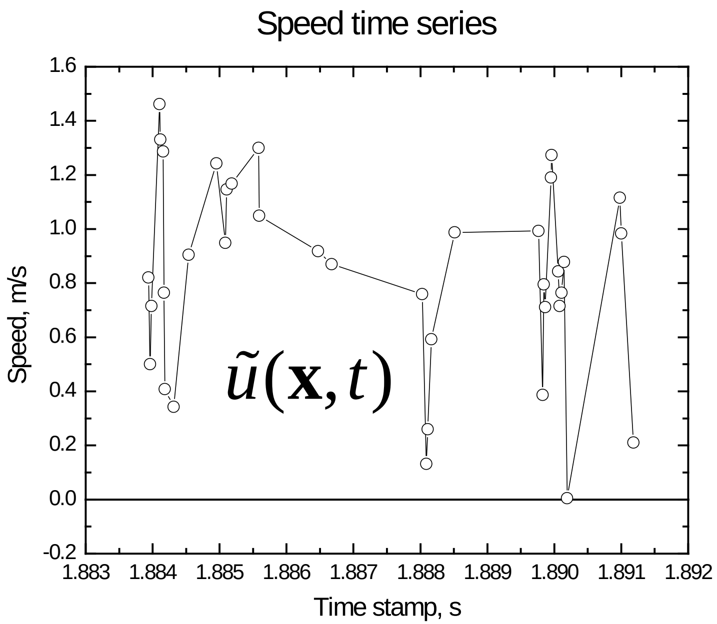


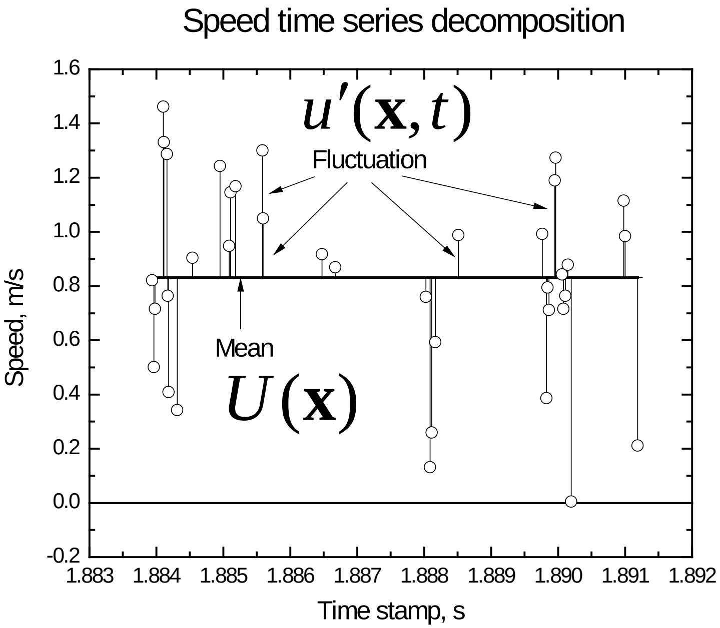
Hydrostatically Tested to 2,000 psi (1,500 psi design P) by FESCO, Ltd.



Turbulence Generation

Nomenclature background

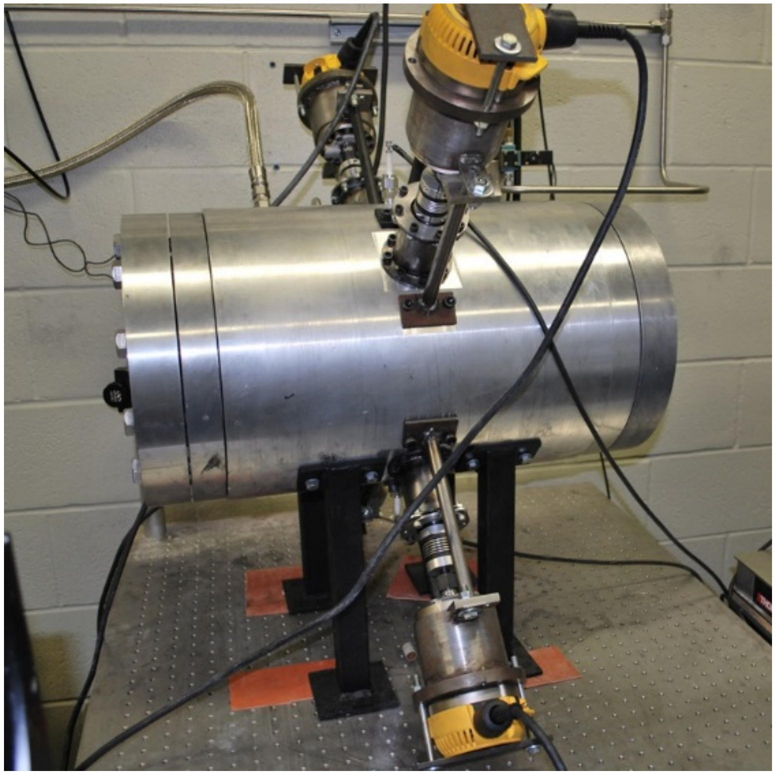


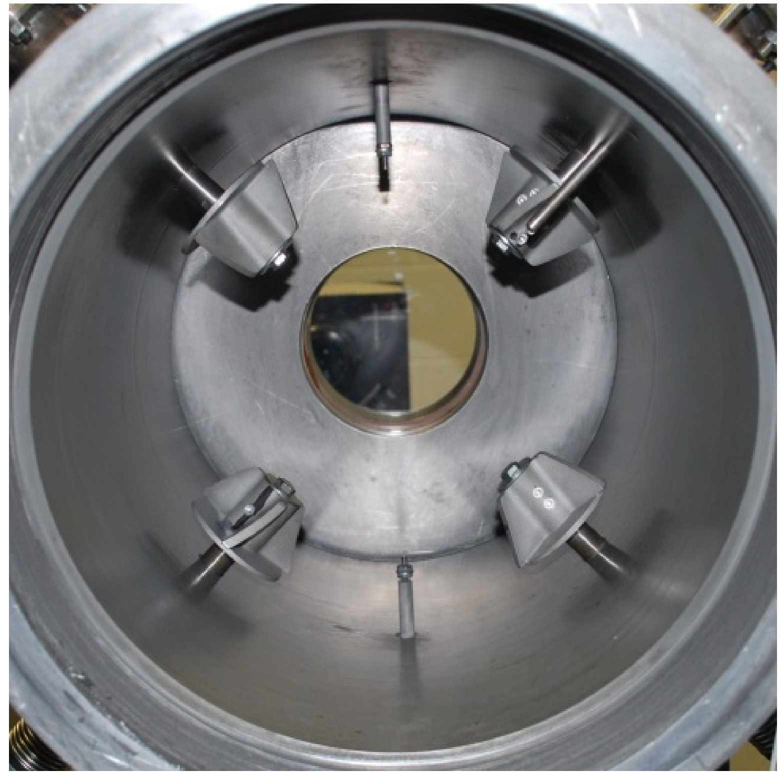


$$\tilde{u}(\mathbf{x},t) = U(\mathbf{x}) + u'(\mathbf{x},t)$$

Background

Previous flame bomb at TAMU



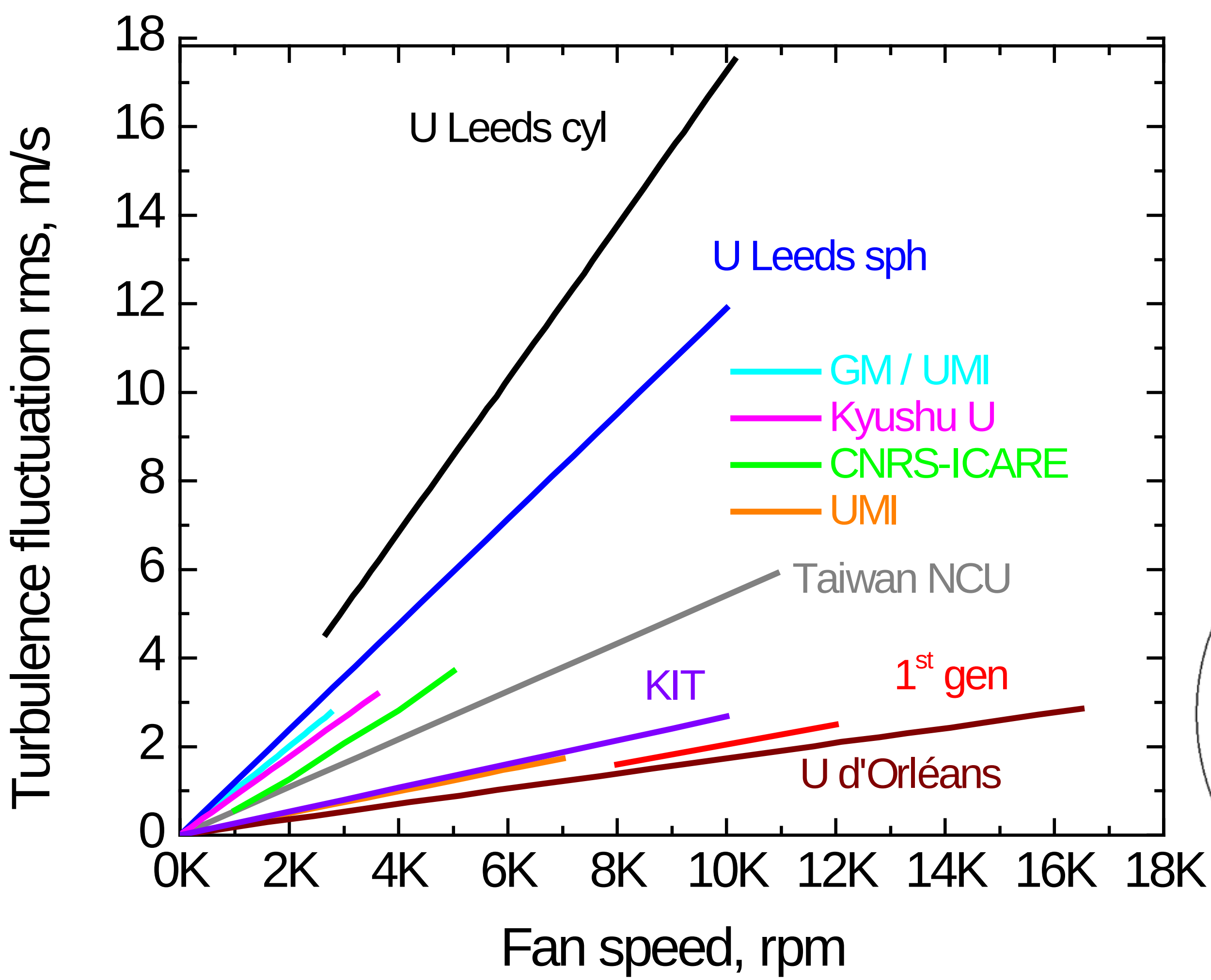


P_{max}	1 atm
ID	305 mm (12”)
L	356 mm (14”)

u_{rms}	1.5 m/s
L_T	27 mm
τ_ε	55 ms

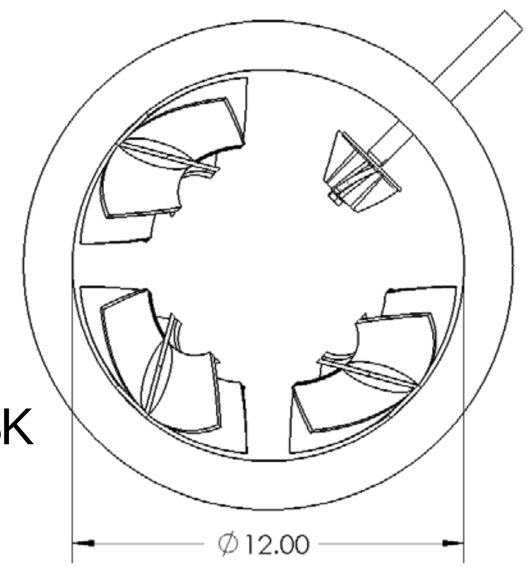
Linear dependence of u' and shaft rpm

Original Fan Design was Not Very Good at Producing Fluctuations



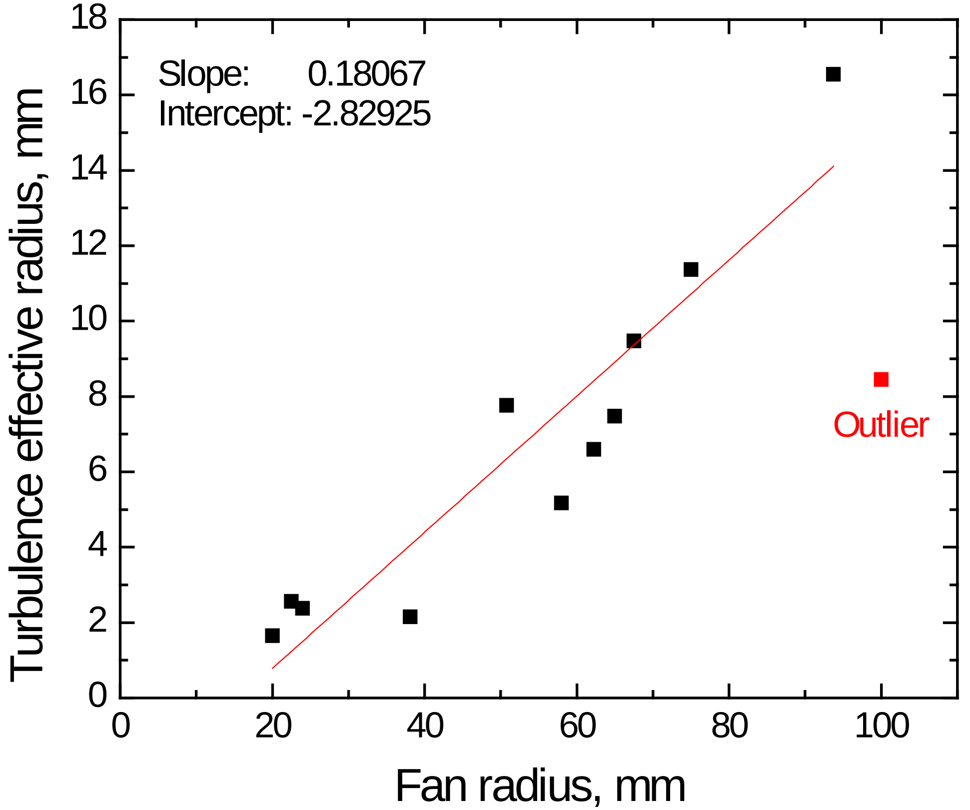
$$u'_{rms} \propto \omega$$

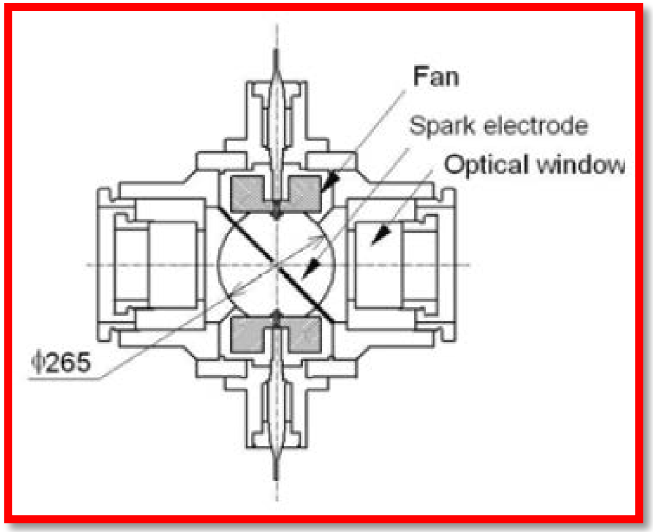
$$u'_{rms} \approx r_{eff}\,\omega$$



Effect of fan size and turbulence

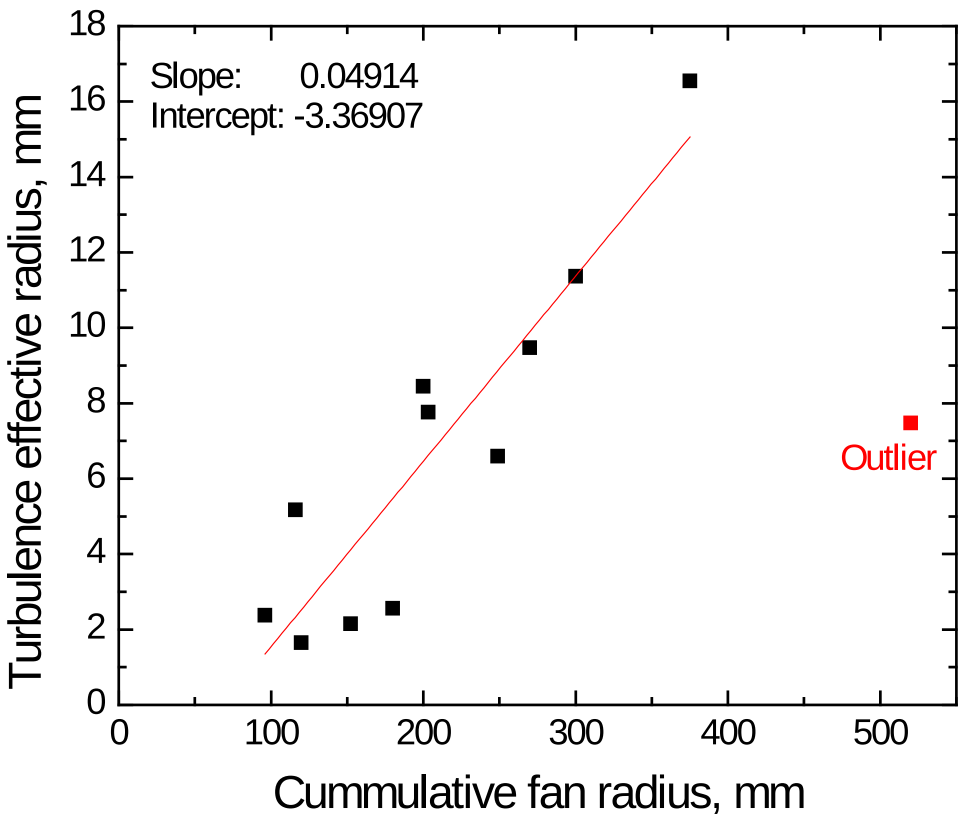
Larger fans are better stirrers. $r_{eff} \approx 0.18\, r_{fan}$

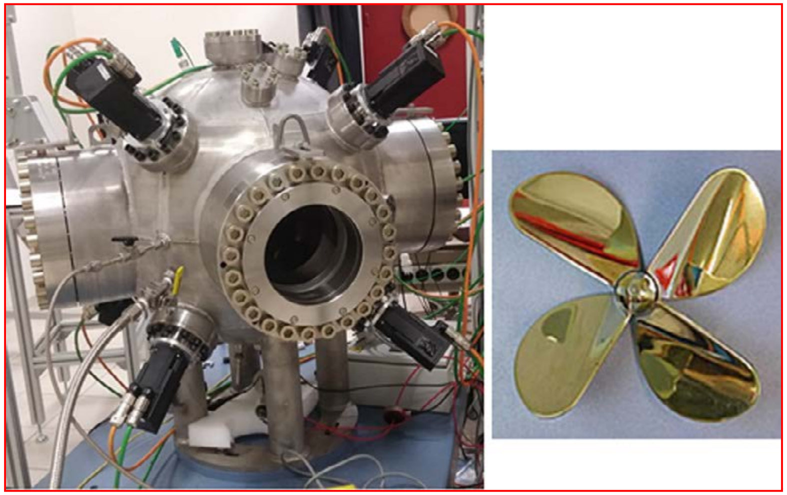




Effect of fan quantity

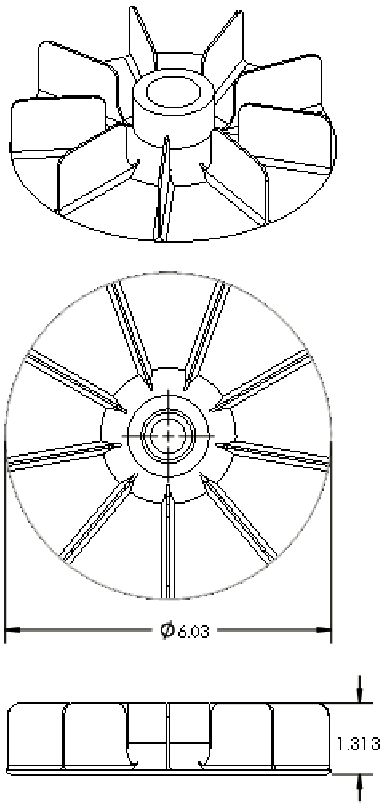
More fans, more vigorous u'_{rms}



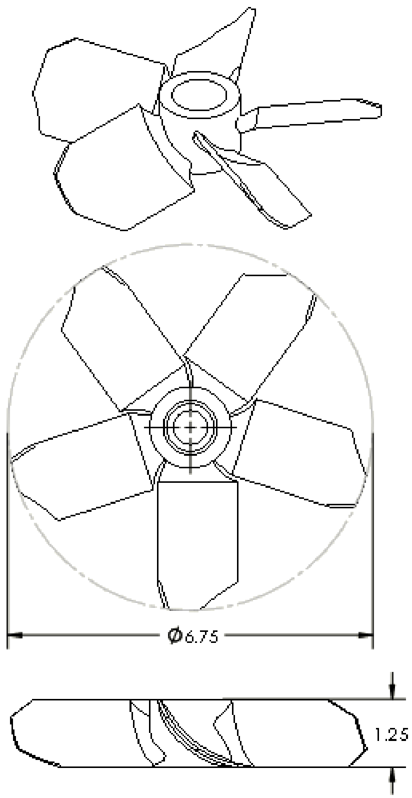


Custom impeller prototypes

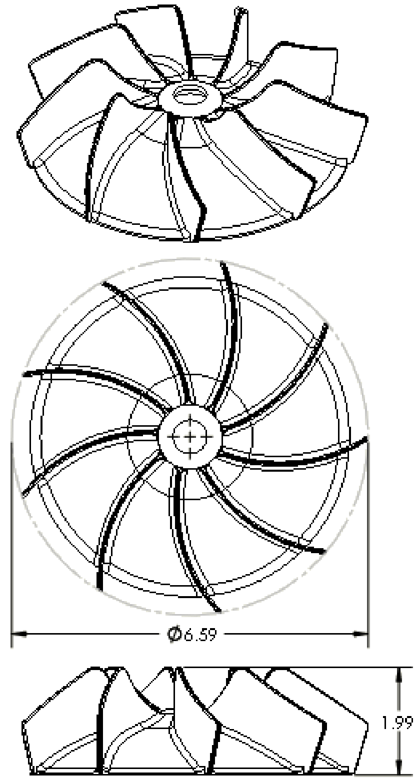
Fan Designs Could be Easily 3D Printed



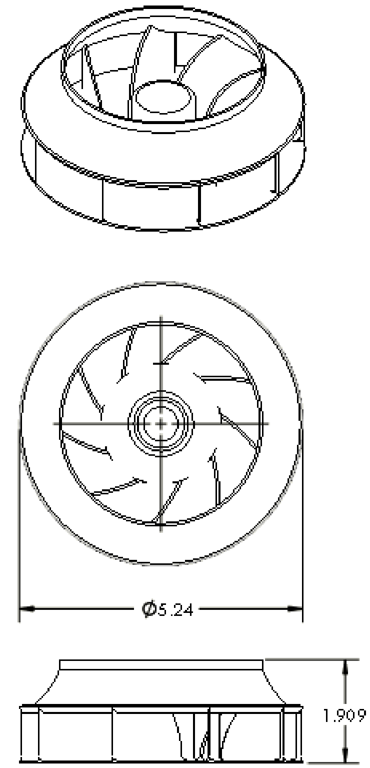
Radial



Axial



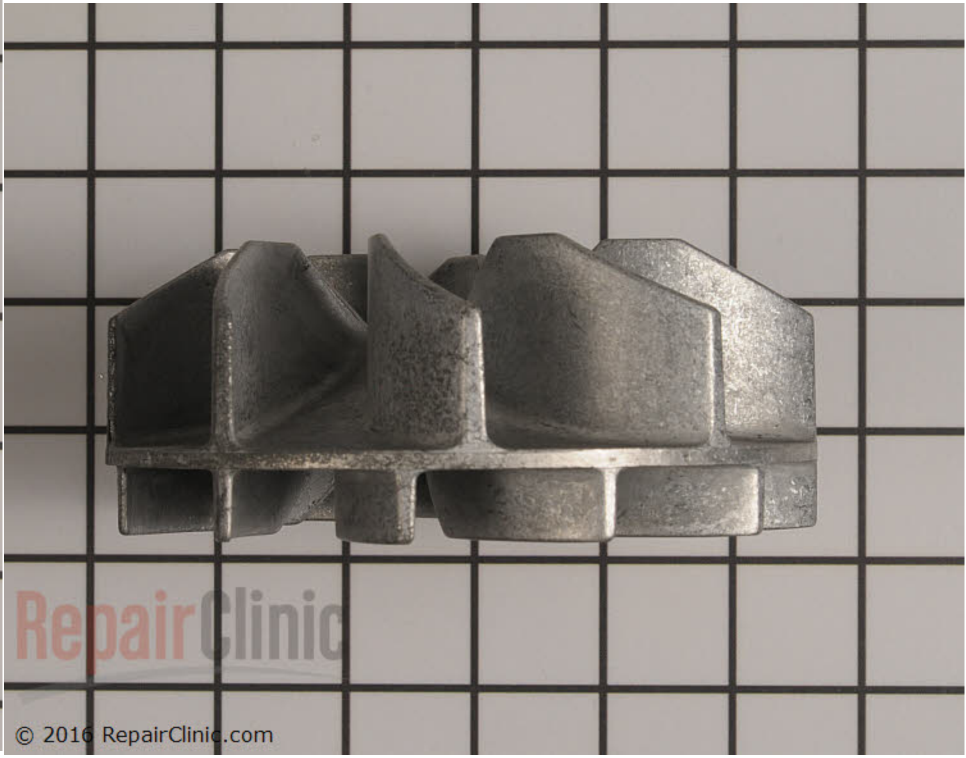
Backward curved



Plug

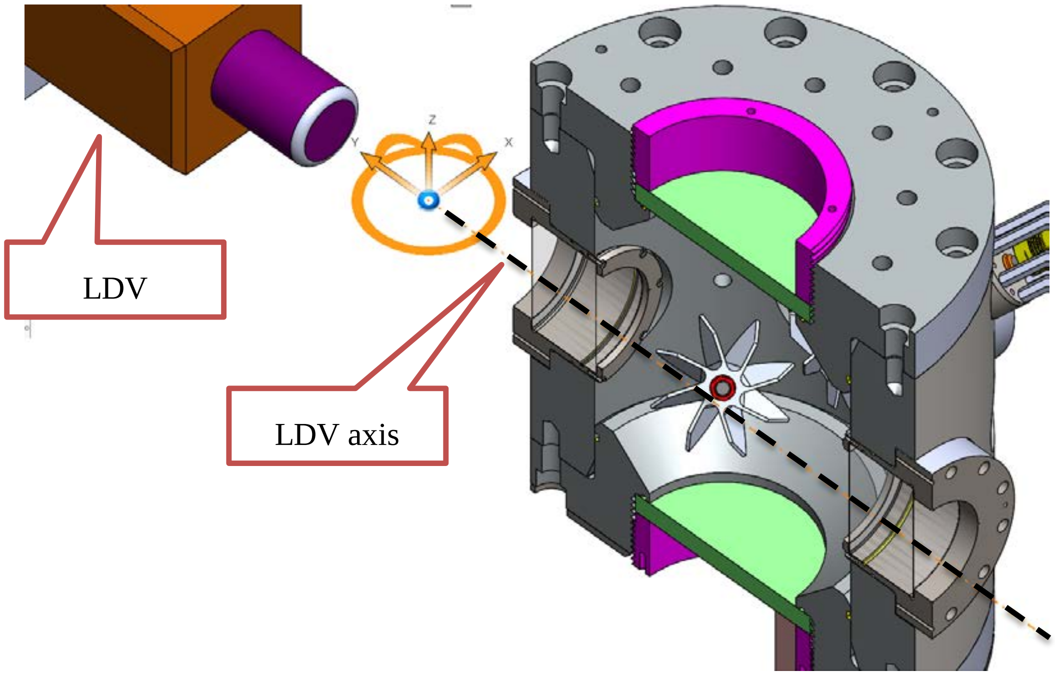
Stock leaf blower impeller

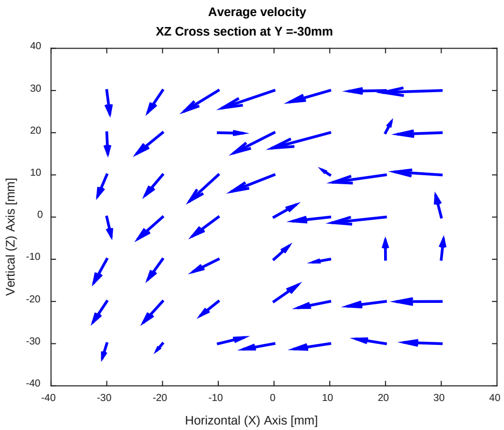
Toro 127-7092, magnesium impeller

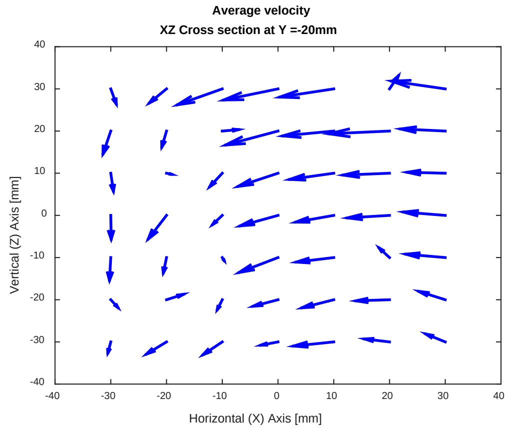


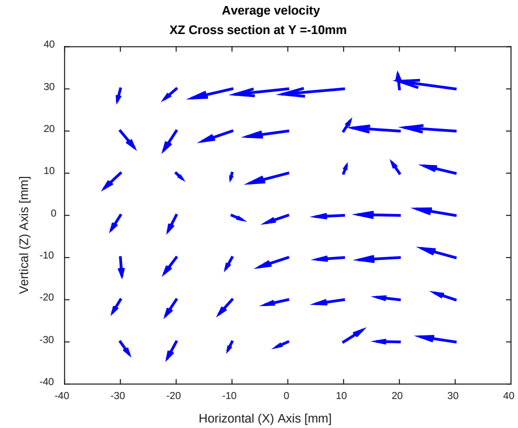
Blower

LDV characterization







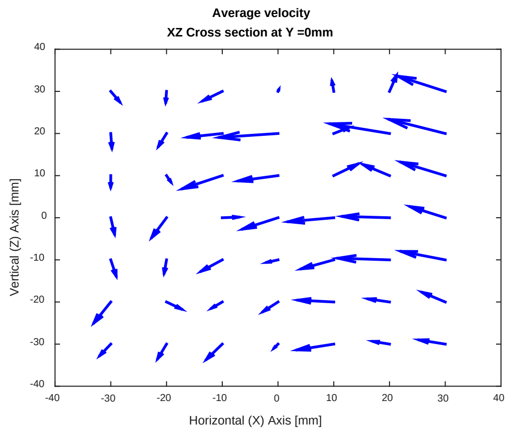


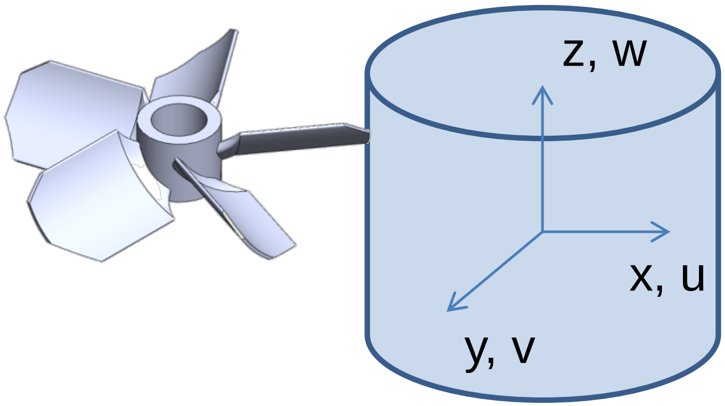
Impeller “A“
1000 rpm

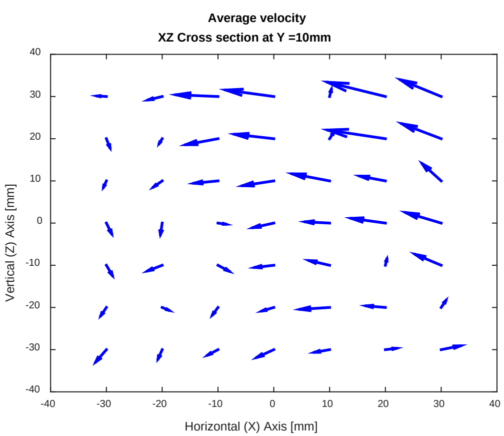
$$\bar{u} = -0.58$$
$$\bar{w} = -0.08$$
$$u_{rms} = 1.52$$
$$w_{rms} = 1.19$$

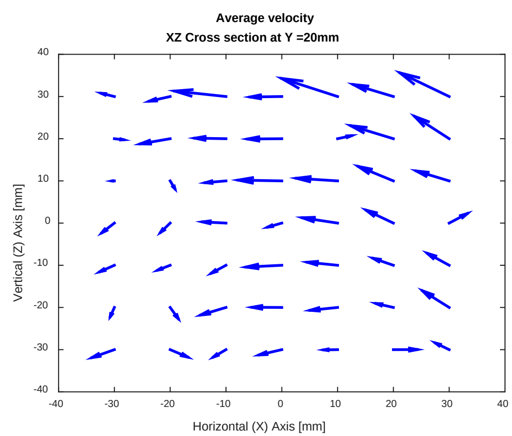
Isotropy = 1.278

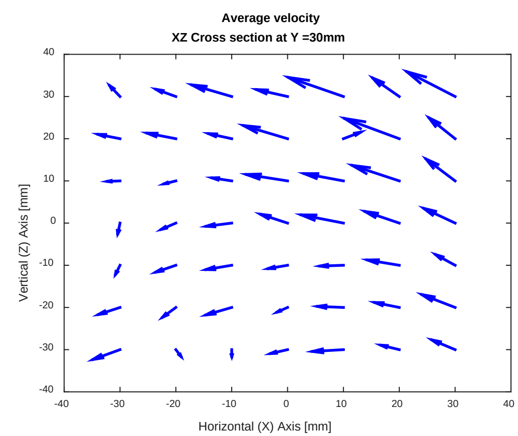
$h_x = 1.00$, $h_y = 1.00$





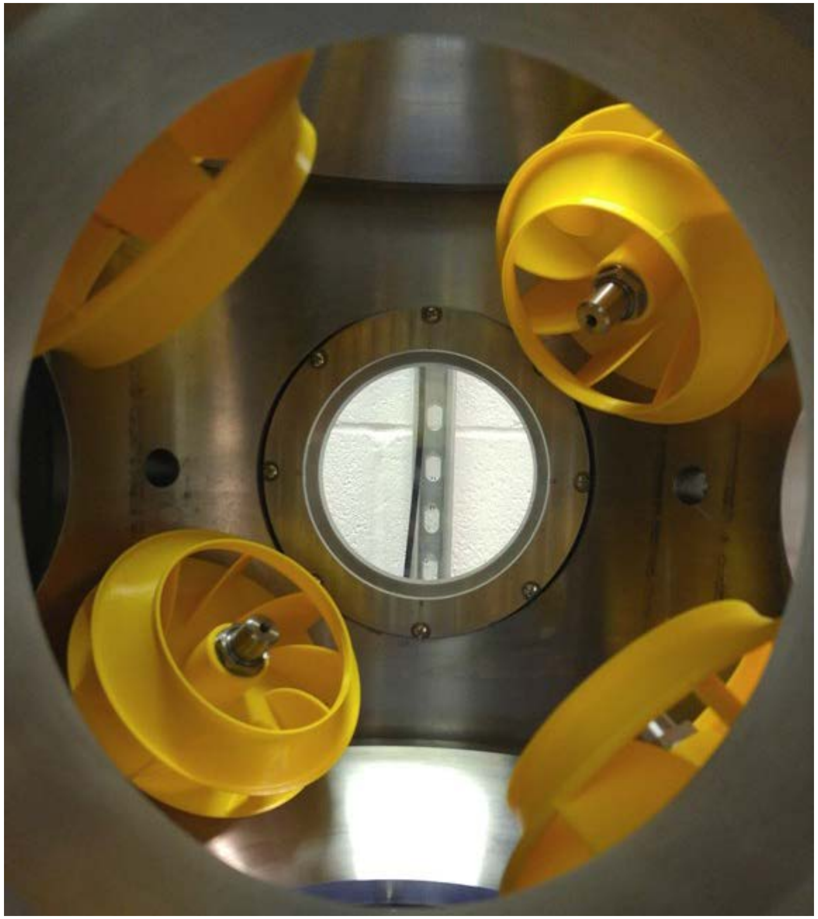


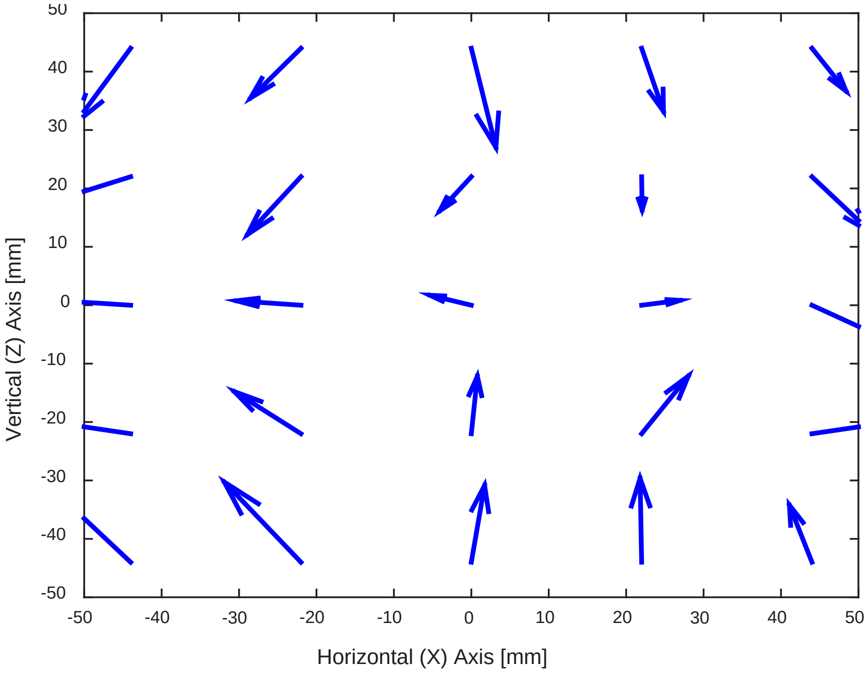




Plug impeller LDV results

Anisotropic turbulence





rpm	2000	4000	6000
Mean velocity C	0.1508	0.4893	1.0823
Turbulence fluctuation c'_{rms}	1.9907	4.1157	6.2090
Inverse intensity C/c'_{rms}	0.0757	0.1189	0.1743
Isotropy u'/w'	0.7600	0.7553	0.7491
Homogeneity std. dev.	0.0827	0.0856	0.0842

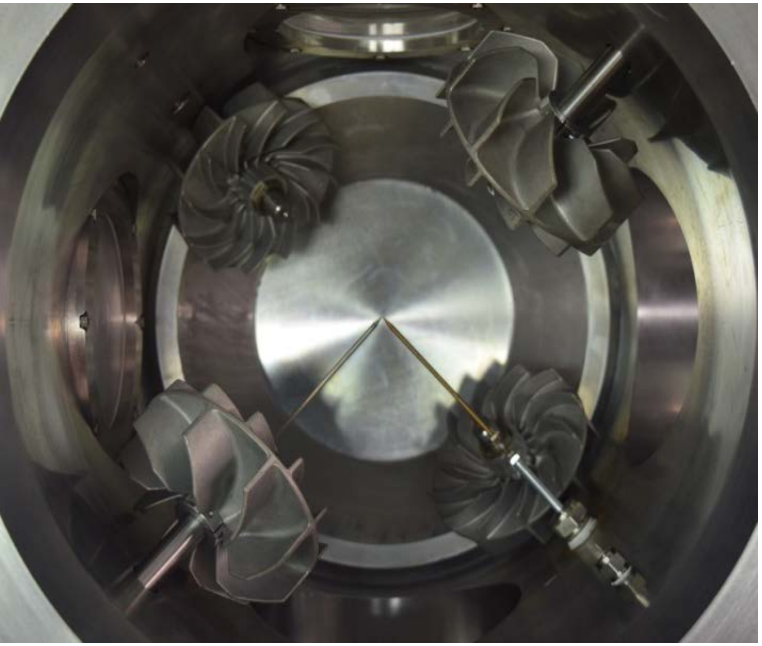
$r_{eff} = 10.07$ mm

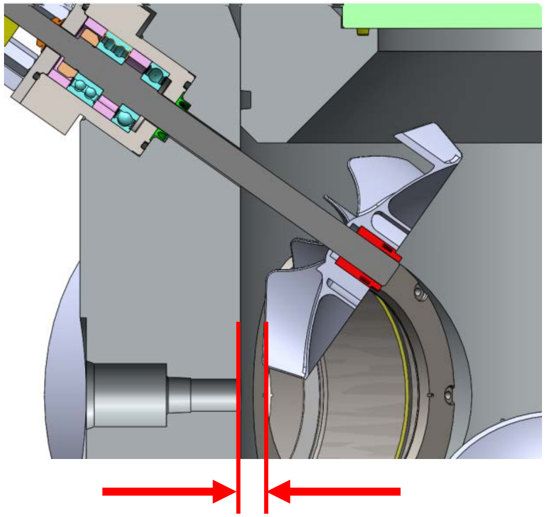
Leaf blower impeller LDV results

The ratio of u'/w' can be influenced

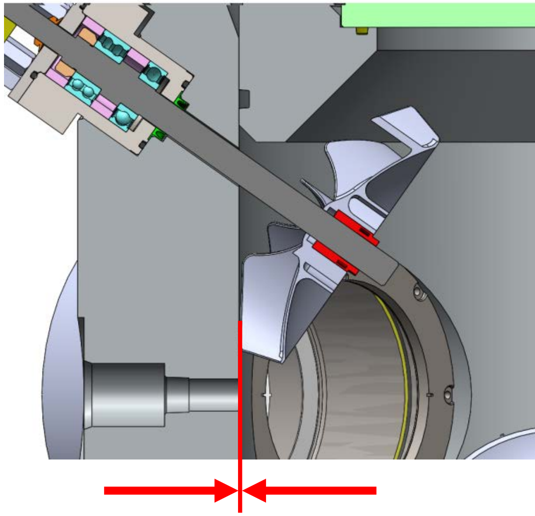
rpm	2000	4000	6000	8000	8000 wall
Mean velocity C	0.2642	0.5646	1.1117	1.1475	1.7777
Turbulence fluctuation c'_{rms}	1.4026	2.7936	4.221	5.5316	5.3769
Inverse intensity C/c'_{rms}	0.1883	0.2021	0.2634	0.2074	0.3306
Isotropy u'/ w'	1.2719	1.2485	1.2786	1.2366	1.0157
Homogeneity std. dev.	0.0957	0.0974	0.1087	0.0971	0.1002

$r_{eff} = 6.6$ mm





Open gap



Close clearance

Task 5 – High-Pressure Turbulent Flame Speed Measurements

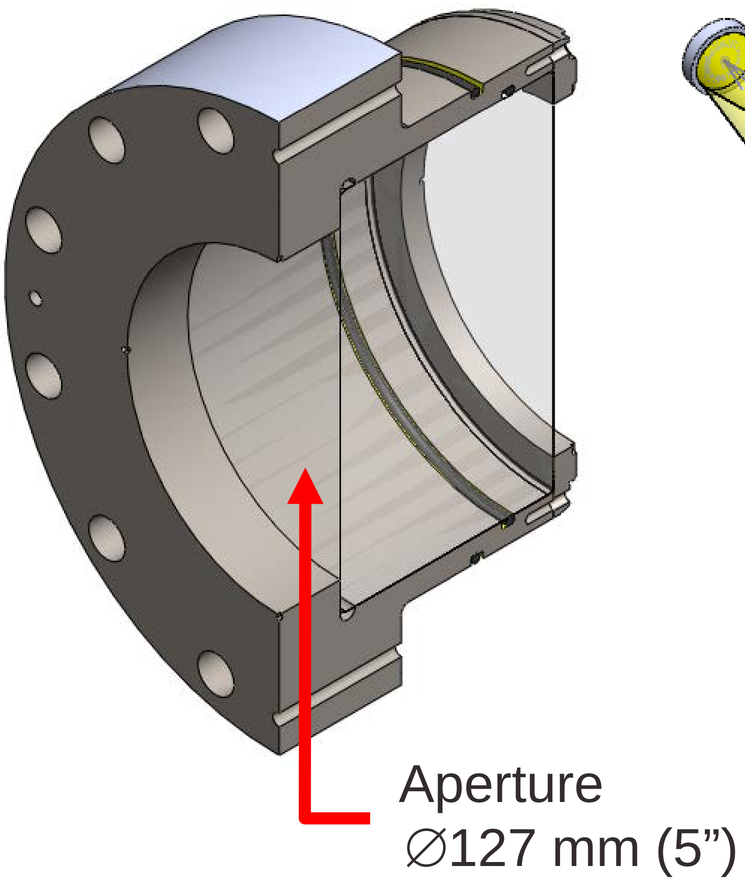
Task 5 – High-Pressure Turbulence

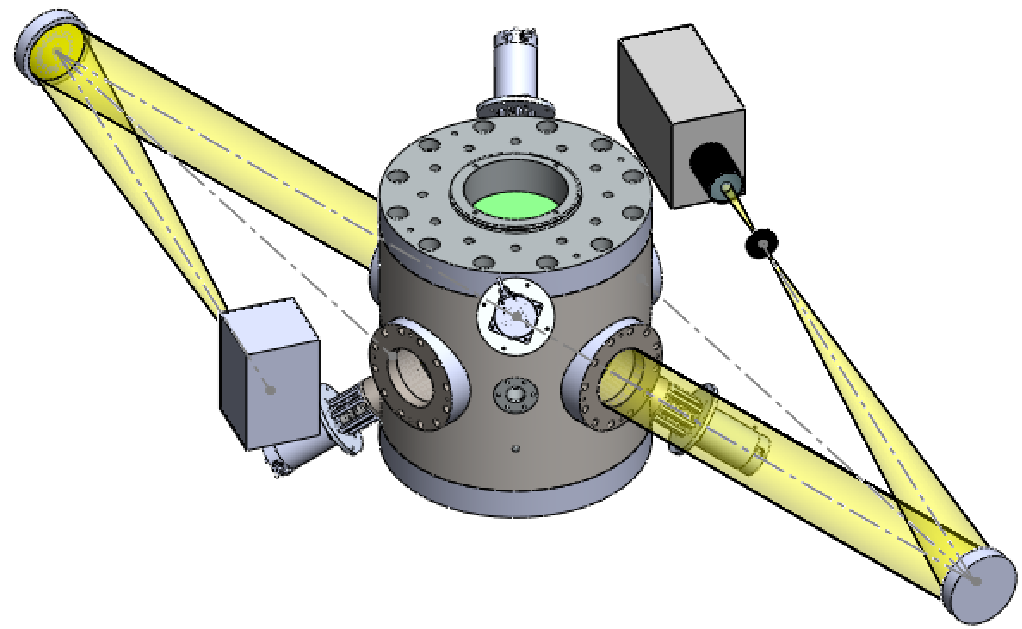
High-Pressure Experiments Were Performed for Selected Syngas Blends

- Hydrogen Characterization Tests, Laminar and Turbulent
- Identify Syngas Blends for Study with Turbulence Generation
- Perform Experiments at Elevated Pressures (10 bar)
- Collect Database of Images and Flame Growth Measurements

Optical access

Schlieren optical diagnostics enabled

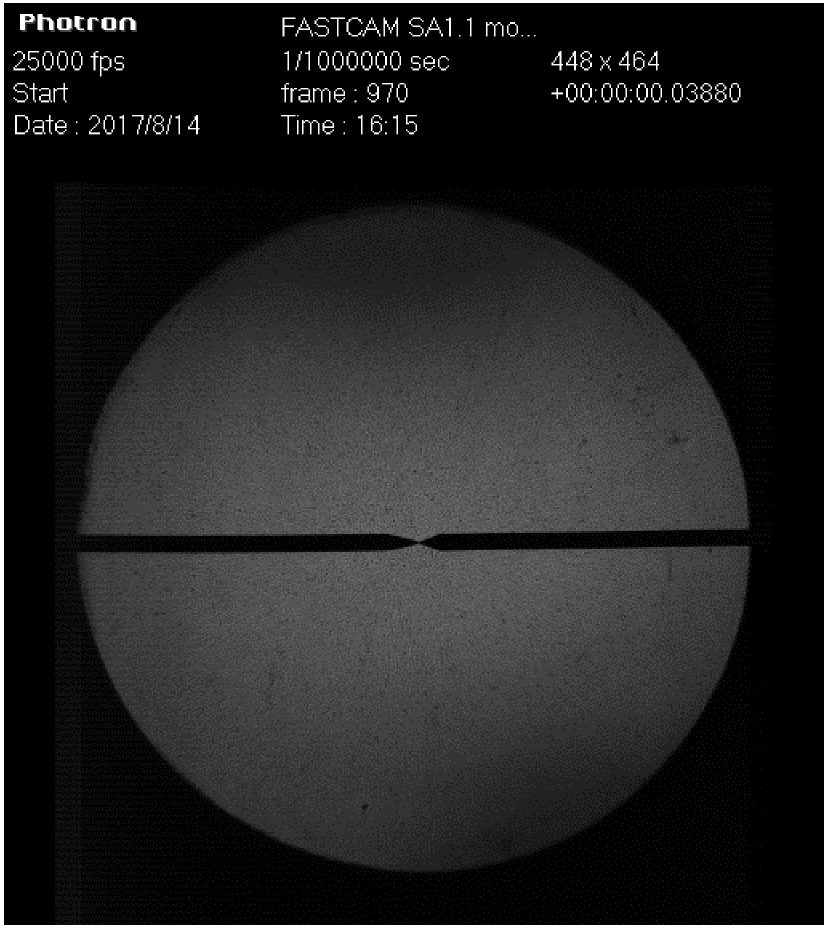




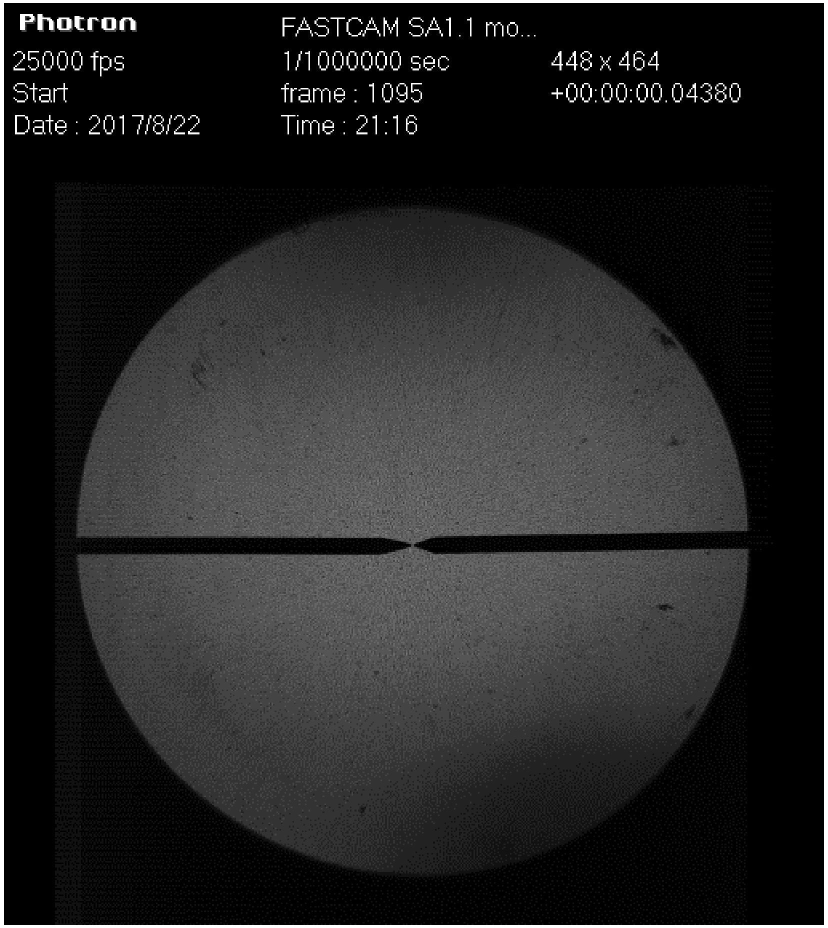
Laminar flame speed

Validation Experiments Performed for H_2

H_2-Air, 10 bar, no fans



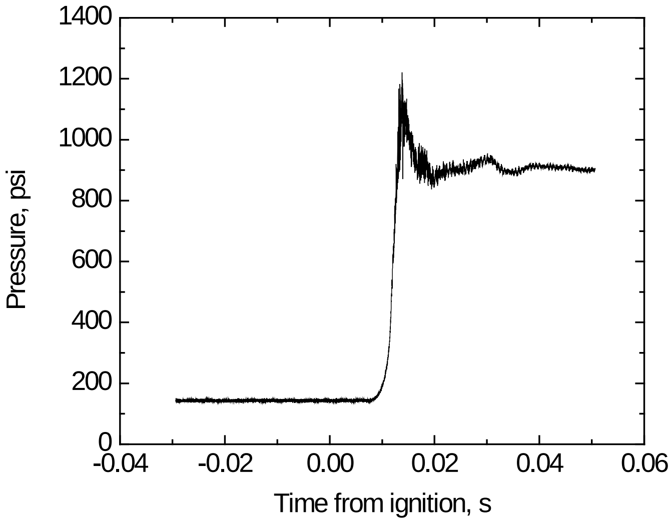
H_2-O_2-He, 10 bar, no fans



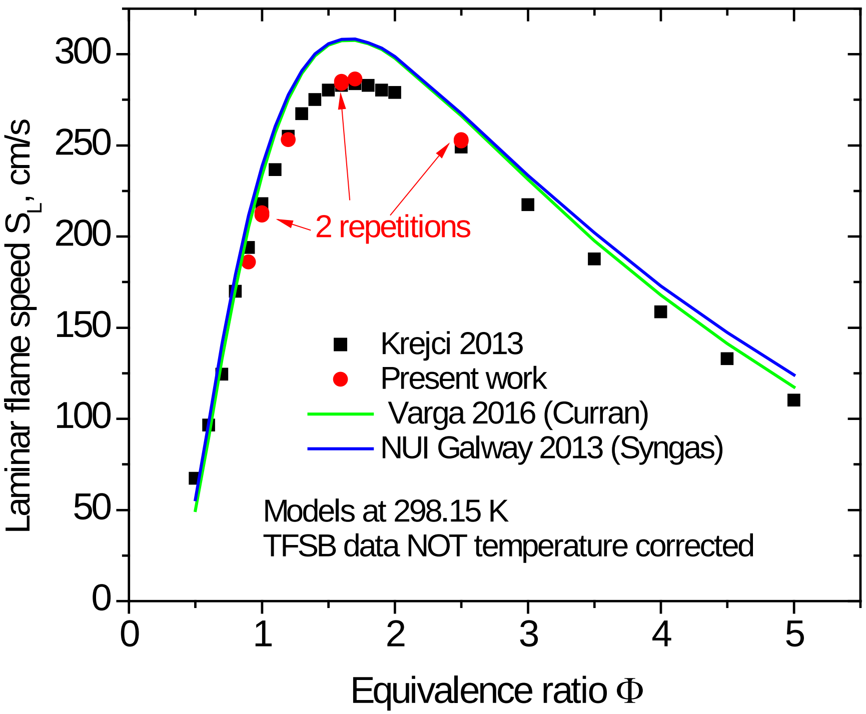
Laminar flame speed validation

Excellent reproducibility and repeatability

Pressure trace of 10 bar run



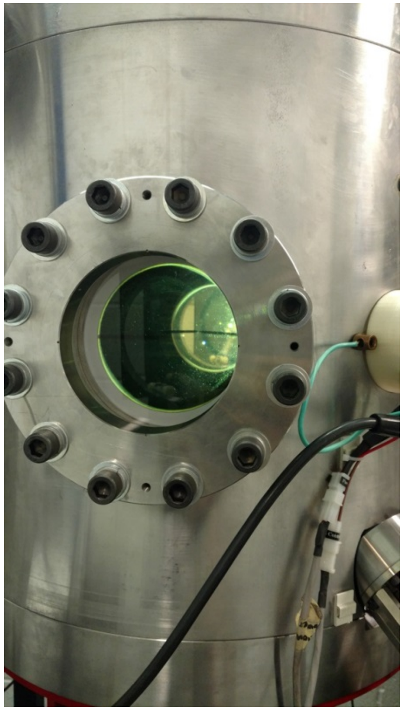
H_2 laminar flame speed, 1 atm



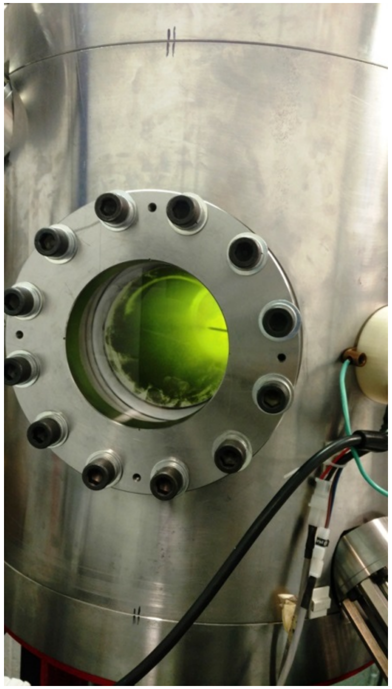
Nitrogen Oxides formation

Unintended wet NOx scrubber

Combustion products immediately after ignition

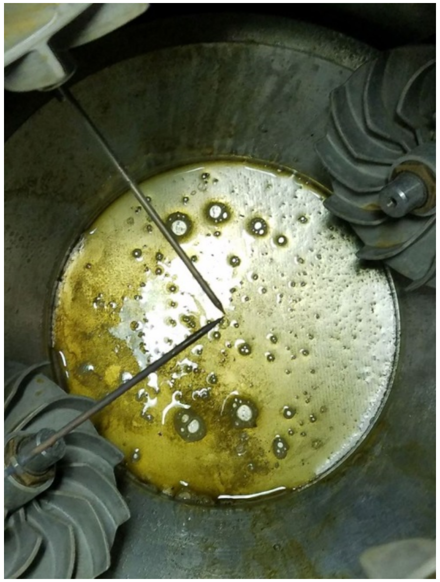


5 bar H_2-air

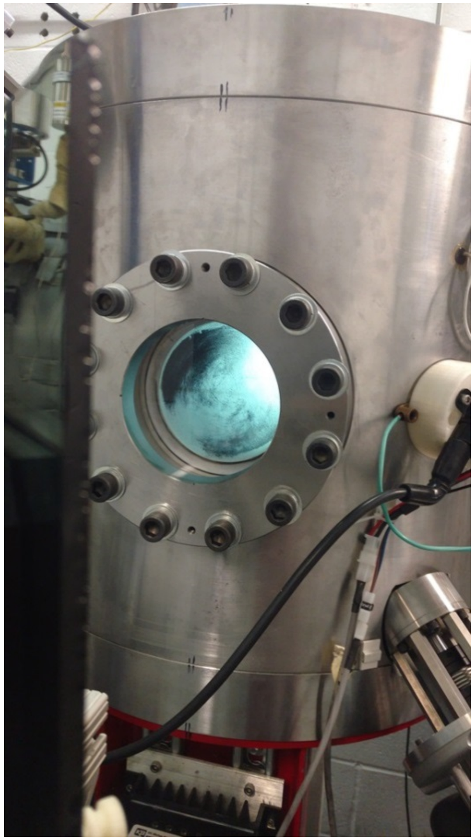


10 bar H_2-air

Condensate after cooldown



10 bar H_2-air



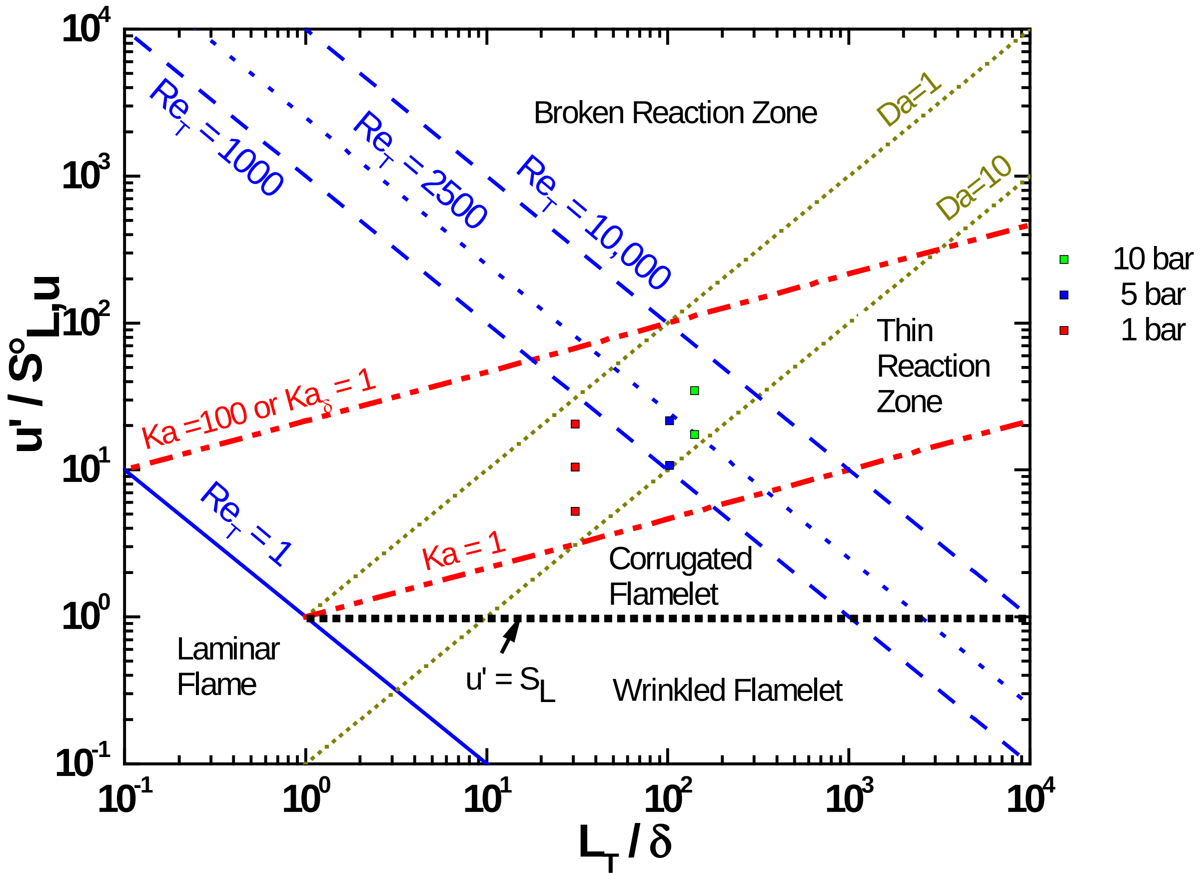
10 bar H_2-O_2+6He

Turbulent experiment matrix

Syngas H_2:CO (50:50), Φ = 0.5, ambient temperature

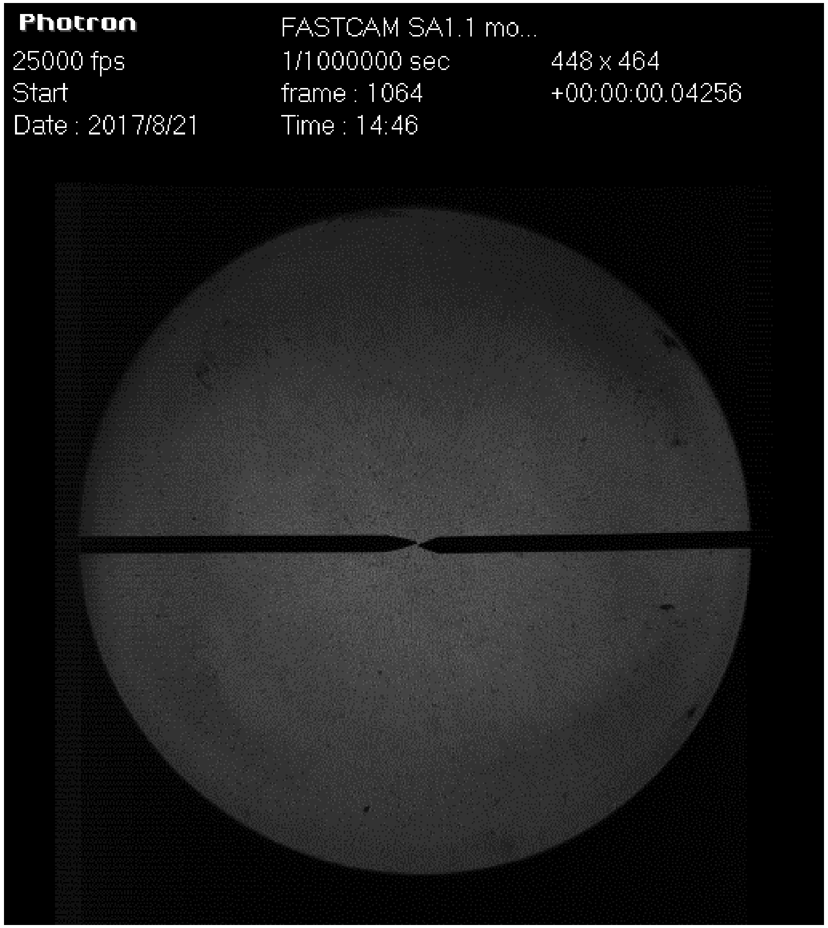
	$S_{L,u}^{\circ}$	δ_L	Re_T		
	m/s	**µm**	**1.4 m/s**	**2.8 m/s**	**5.5 m/s** ← u′
1 bar	0.269	649	1621	3242	6369
5 bar	0.130	195	8116	16,231	
10 bar	0.081	142	16,185	32,370	

Borghi diagram

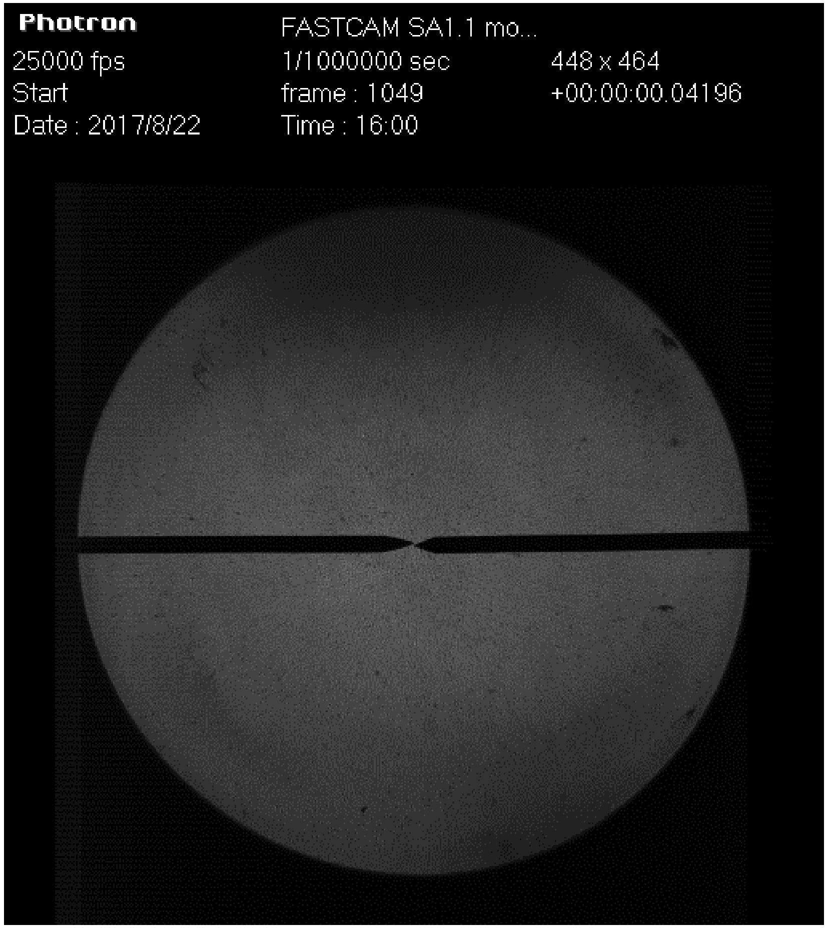


Turbulent flame speed: 8000 rpm

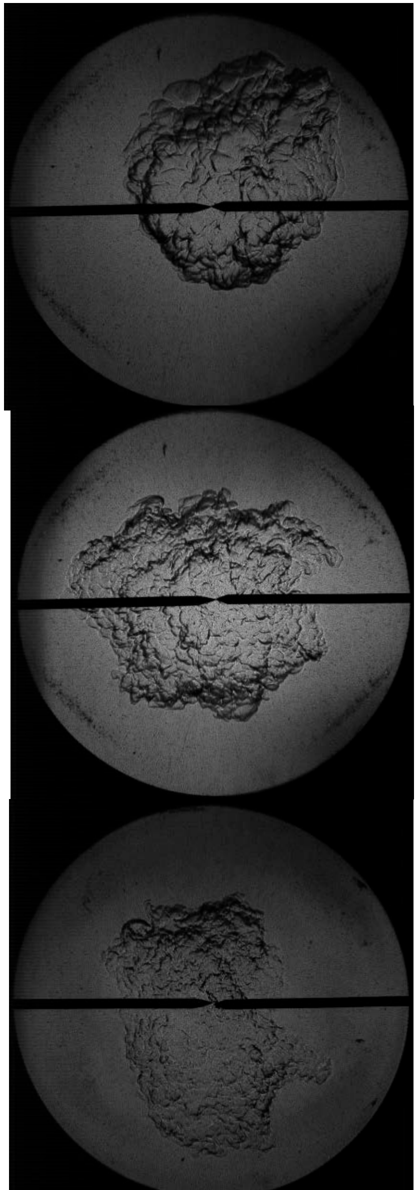
1 bar, 8000 rpm



2 bar, 8000 rpm



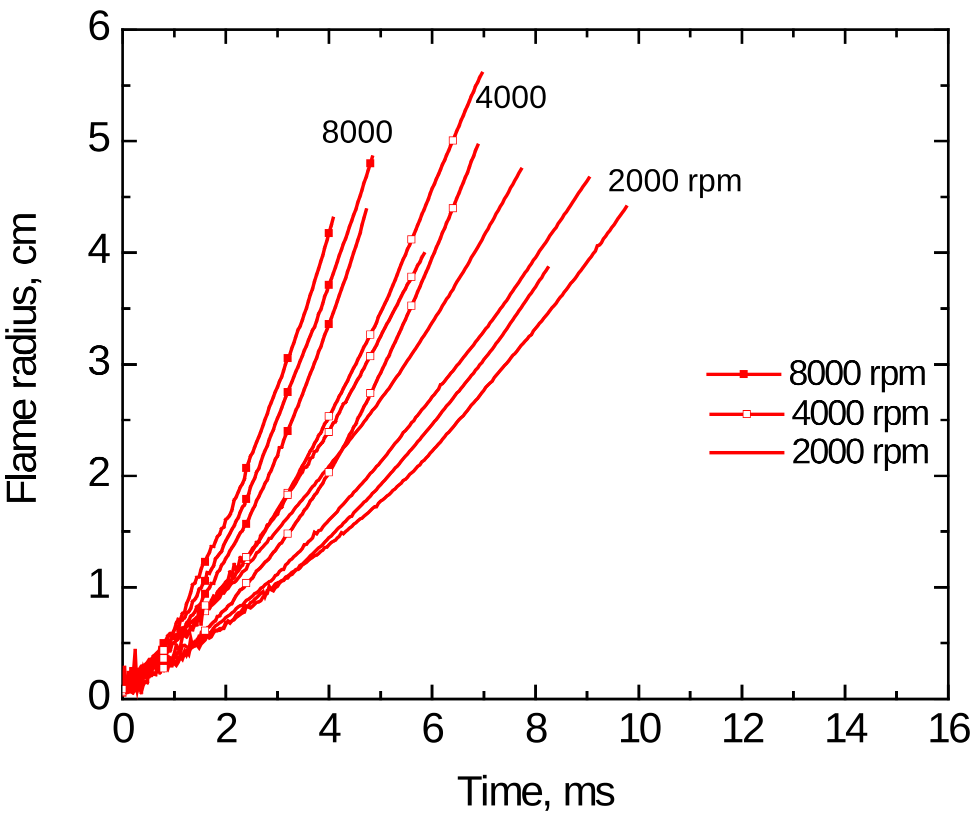
Turbulent flame speed: 1 bar



2000 rpm

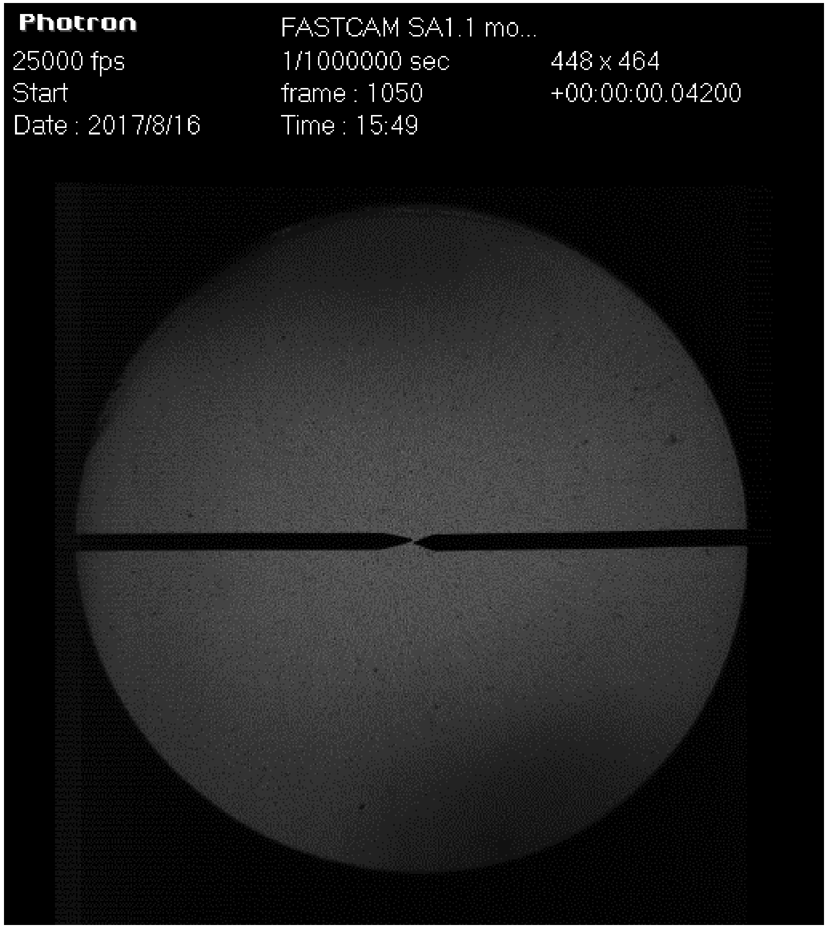
4000 rpm

8000 rpm

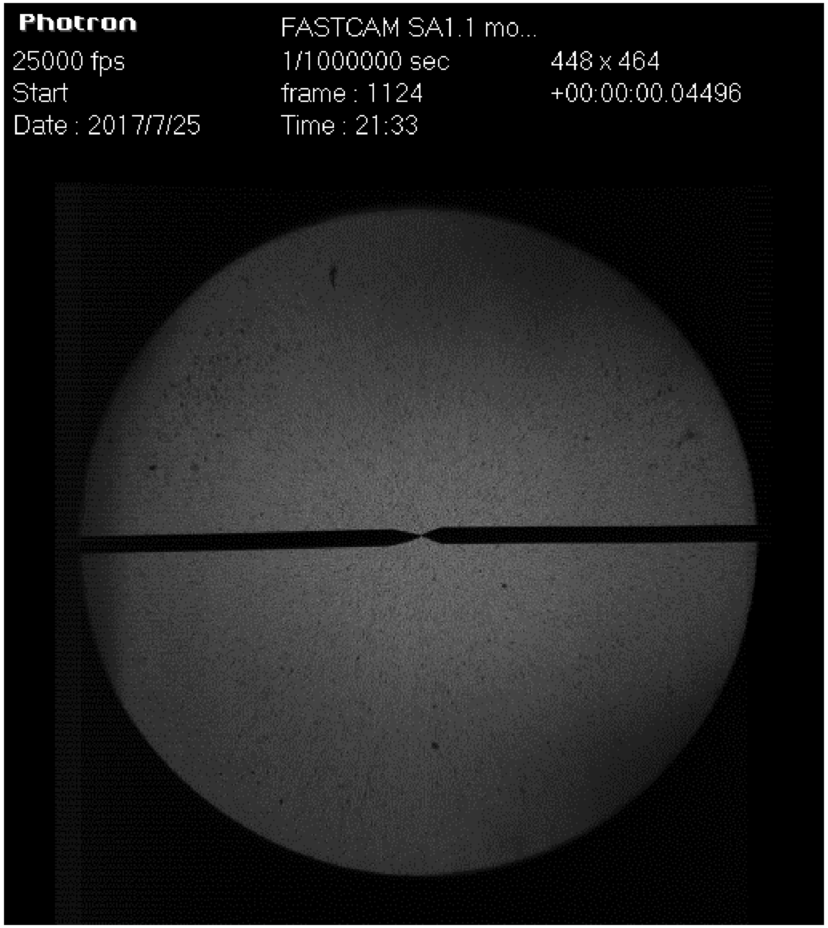


Turbulent flame speed: 5 bar

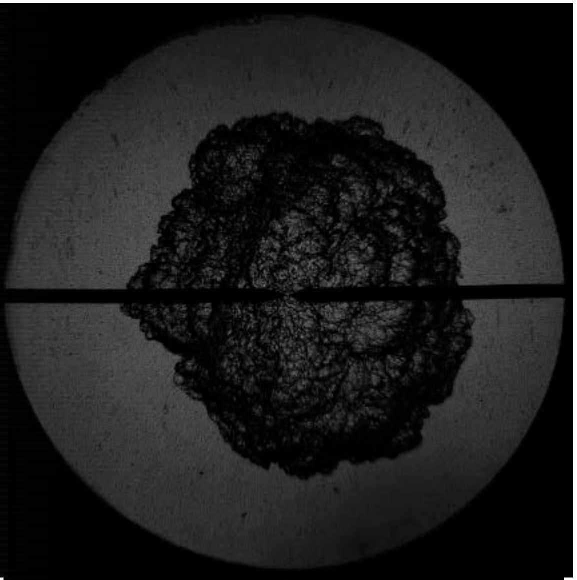
5 bar, 2000 rpm



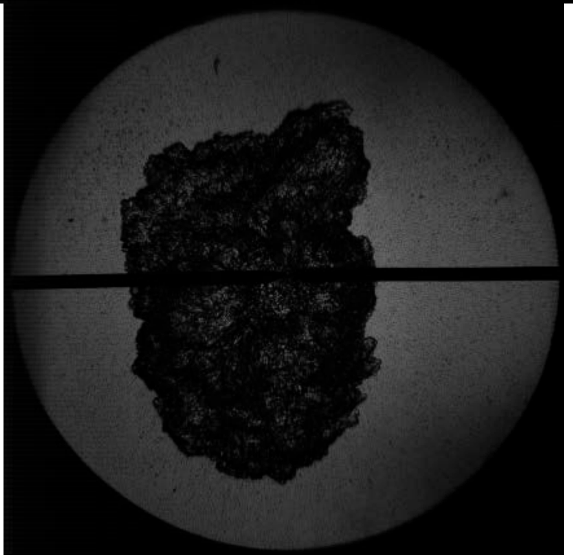
5 bar, 4000 rpm



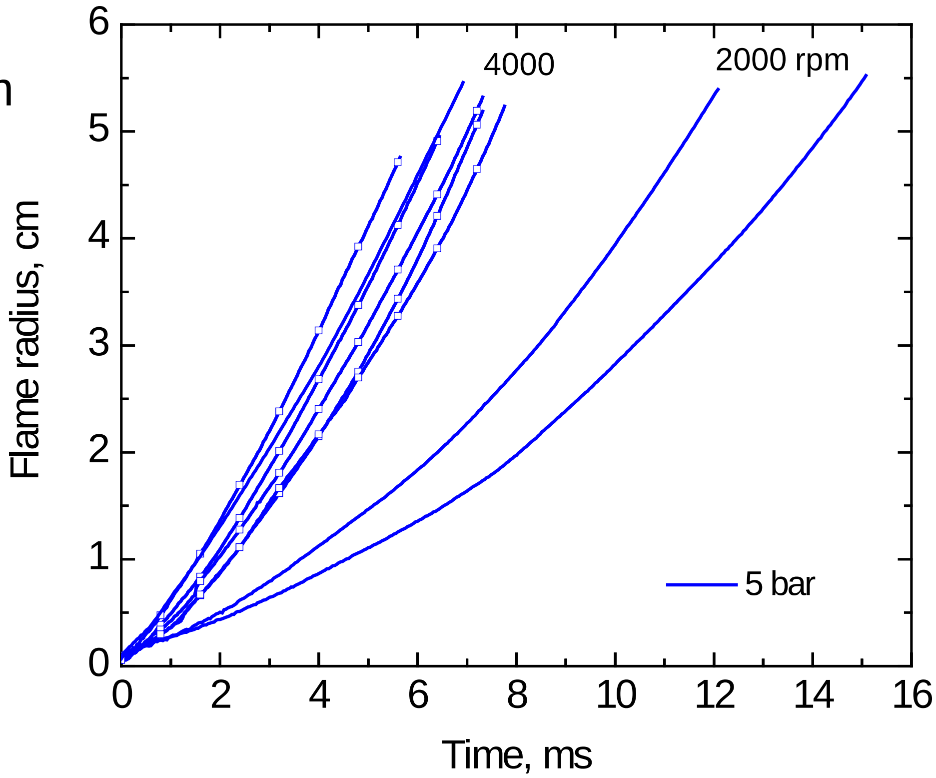
Turbulent flame speed: 5 bar



2000 rpm

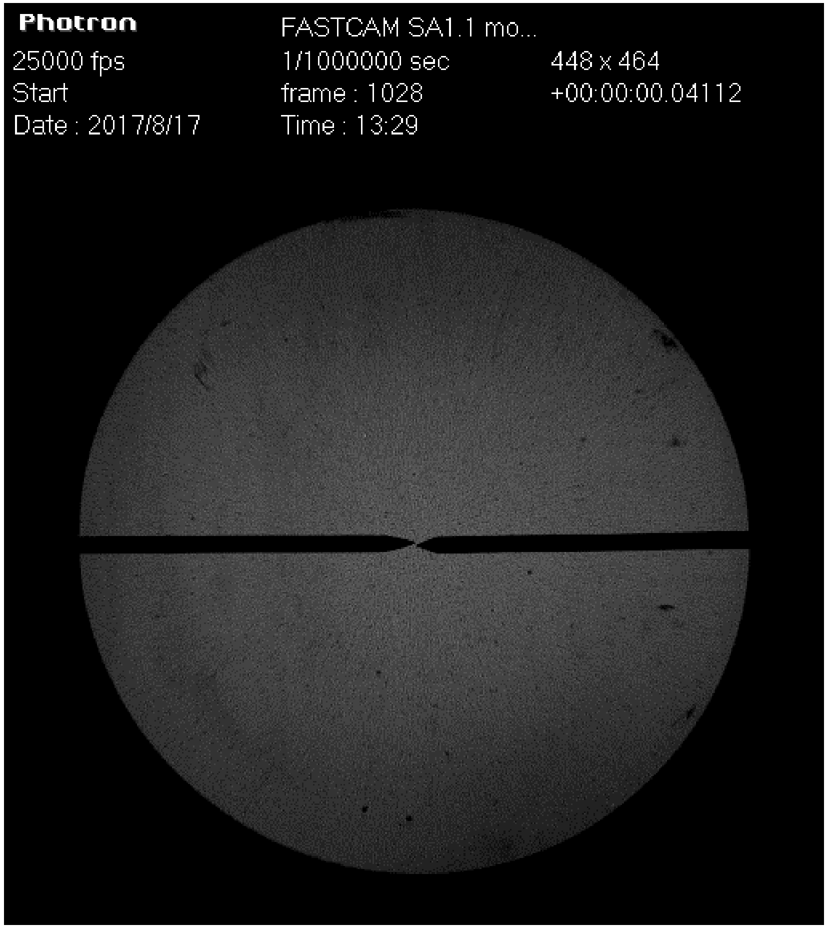


4000 rpm

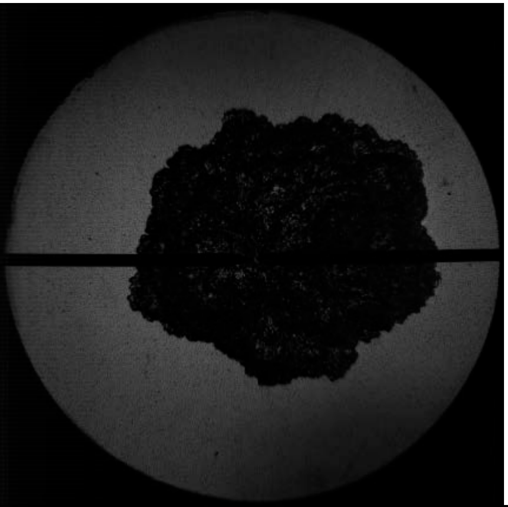


Turbulent flame speed: 10 bar

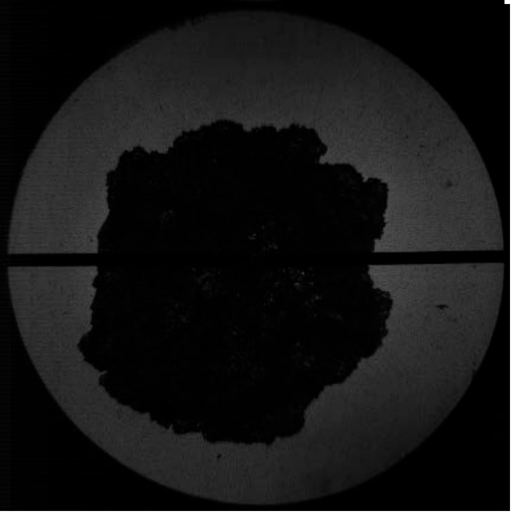
10 bar, 4000 rpm



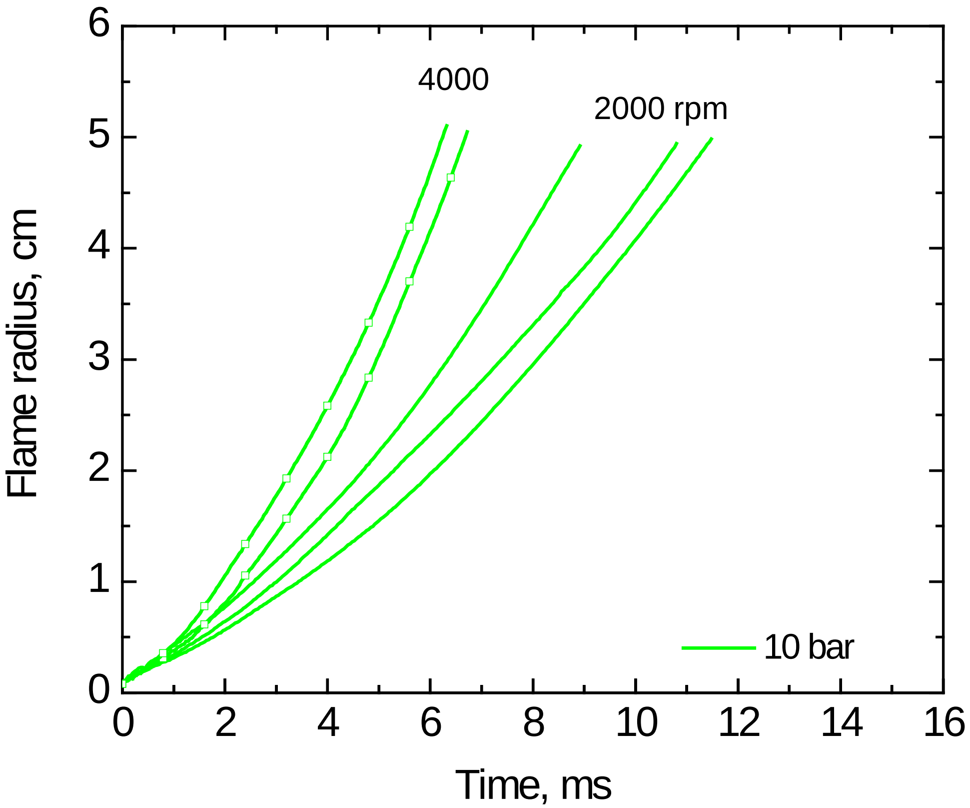
Turbulent flame speed: 10 bar



2000 rpm

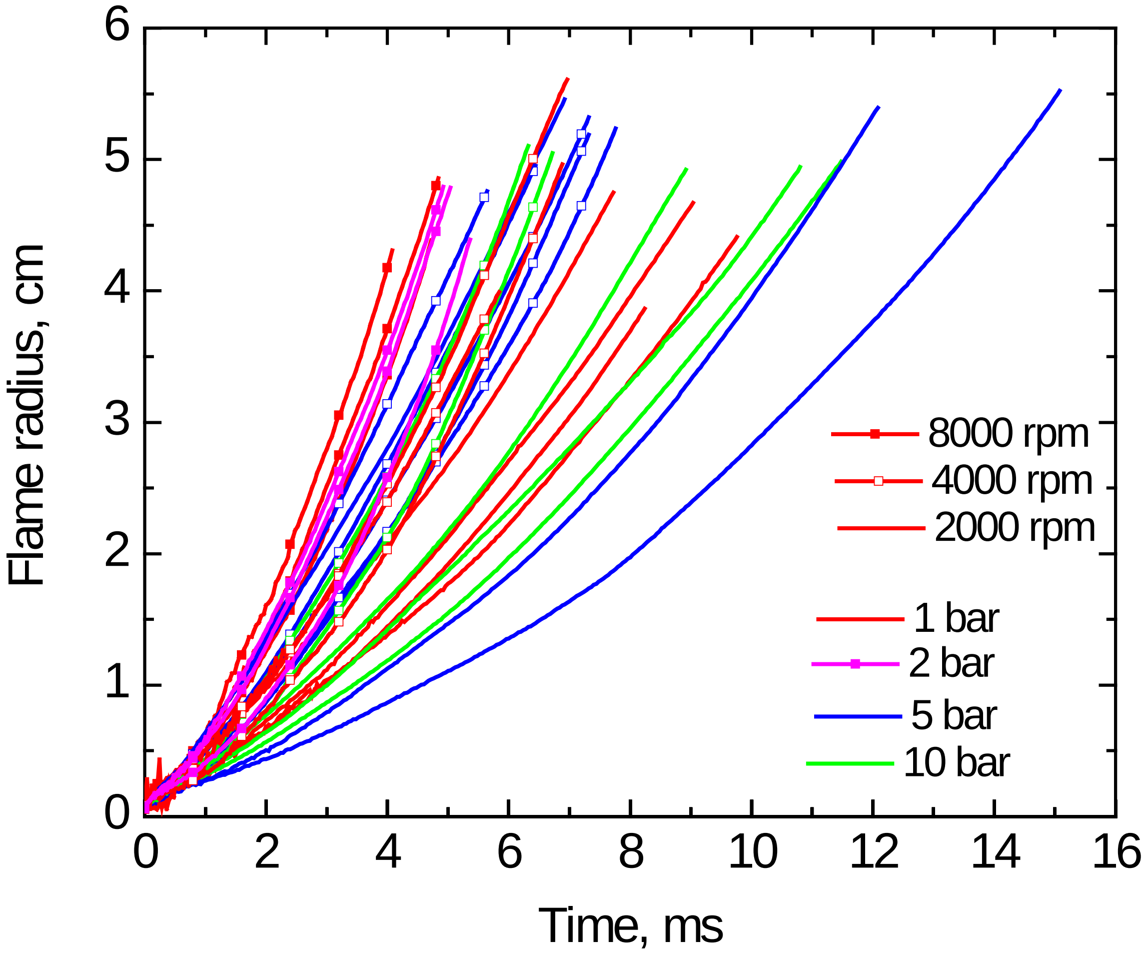


4000 rpm

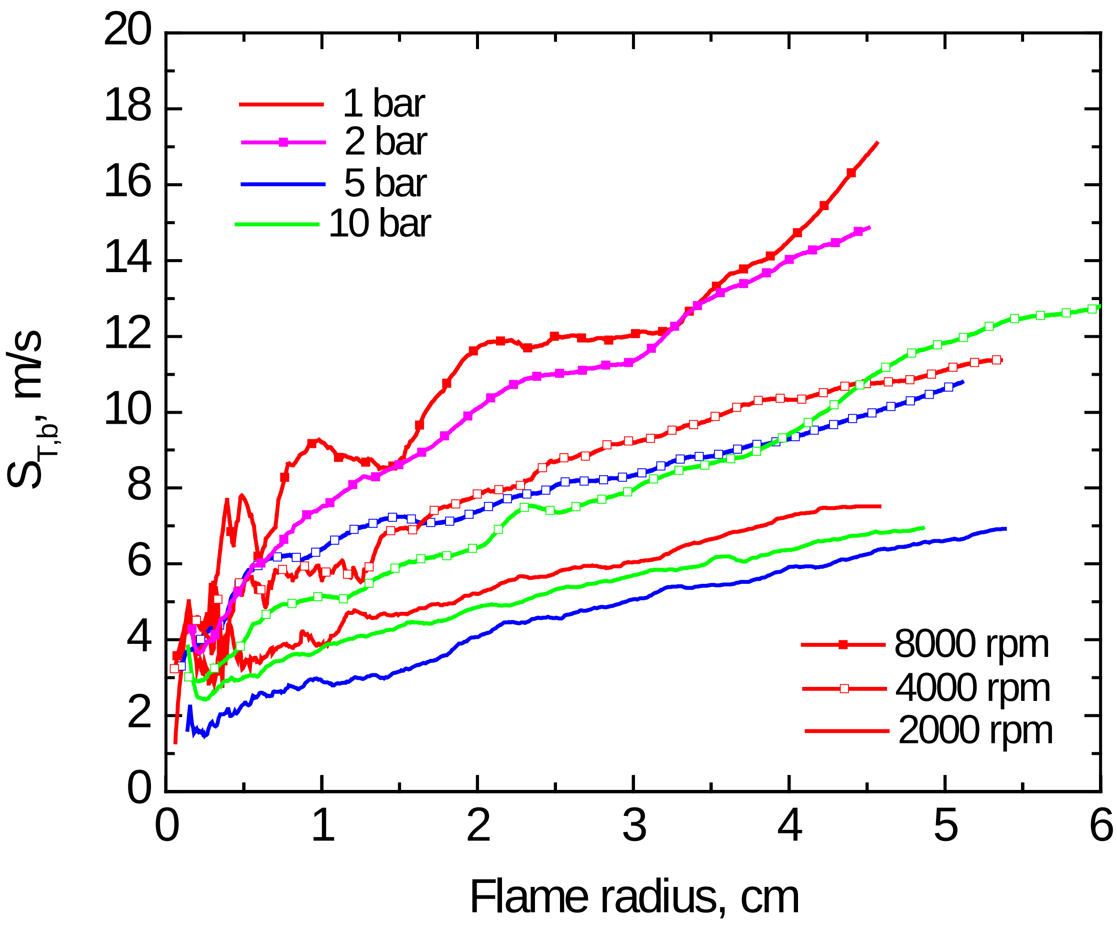


Turbulent flame speed radius

u' is the most determinant factor



Displacement velocity of the burned gas



High-pressure flames

CH_4, Φ=0.9 at 1 & 10 bar

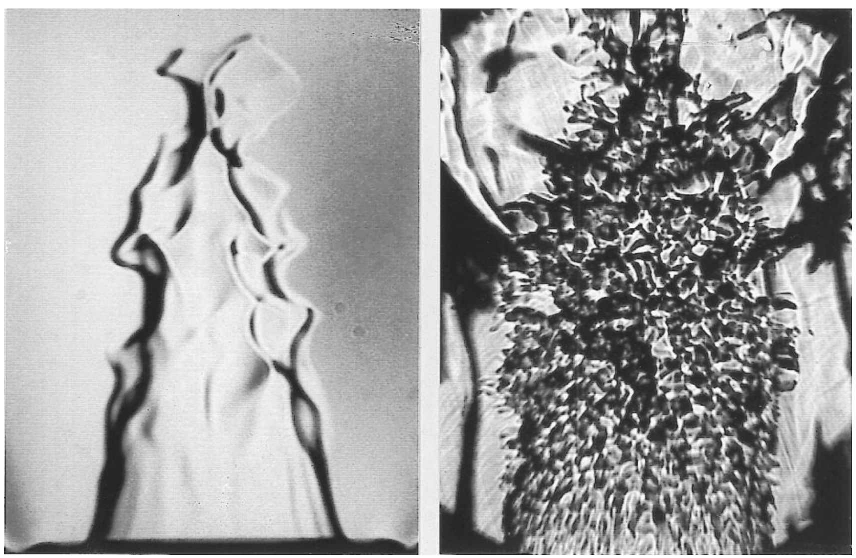
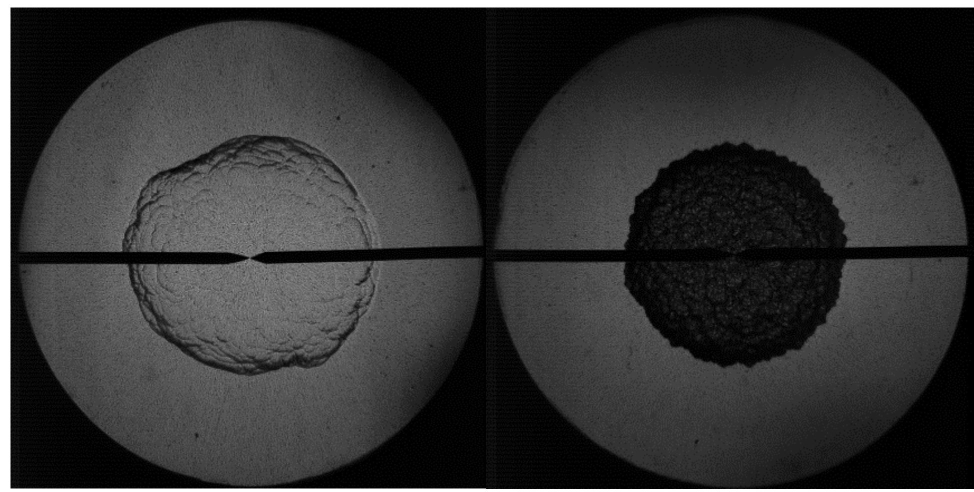


Figure reproduced from (Kobayashi, Tamura et al. 1996)

H_2, Φ=0.5 at 1 & 10 bar



Milestones

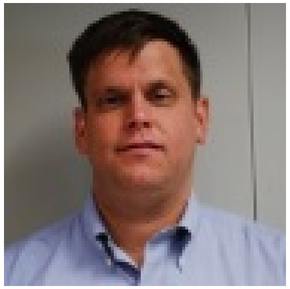
- A new bomb was designed and tested
- u'_{rms} increased from 1.5 to 5.5 m/s
- 10-bar experiments were achieved
- Maximum steady state temperature raised to 400 K
- Blast room was remodeled
- New shared schilieren was implemented
- Results for CO/H_2 mixtures obtained

Project Personnel

TAMU Work is a Team Effort of Several People

Dr. Olivier Mathieu

Charles Keesee



Anibal Morones

Clayton Mulvihill

Summary

Five Main Work Tasks for the Project are Completed

Task 1 – Project Management and Program Planning

Task 2 – Turbulent Flame Speed Measurements at Atmospheric Pressure

Task 3 – Experiments and Kinetics of Syngas Blends with Impurities

Task 4 – Design and Construction of a High-Pressure Turbulent Flame Speed Facility

Task 5 – High-Pressure Turbulent Flame Speed Measurements

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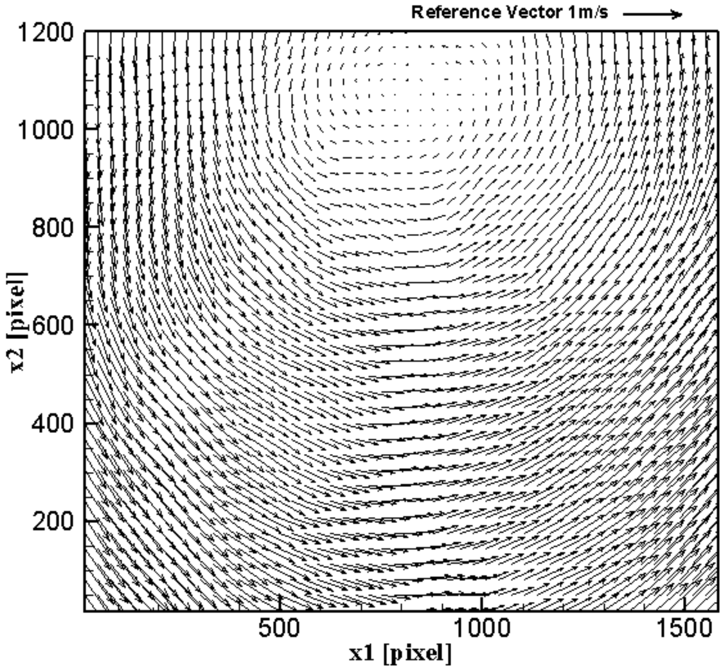
LDV turbulence measurements

Main features of flow ratified with LDV

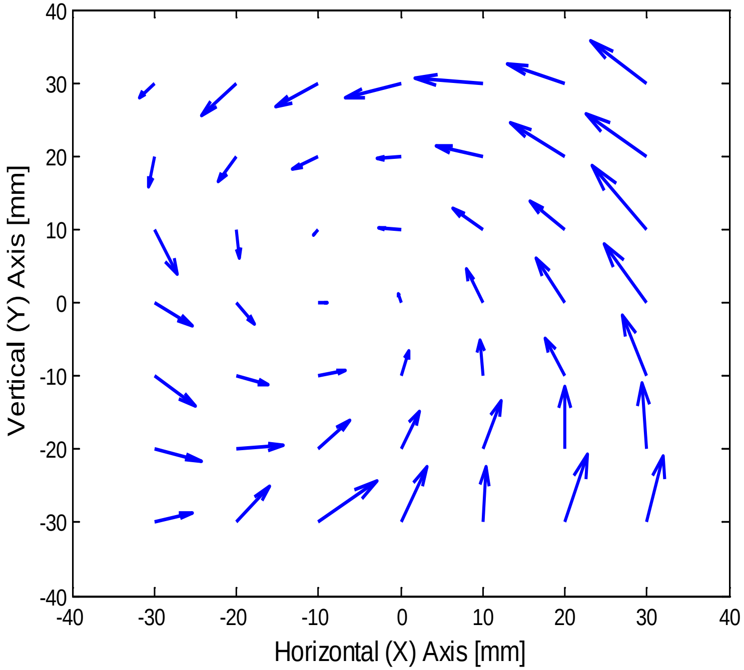
Alpha, PIV

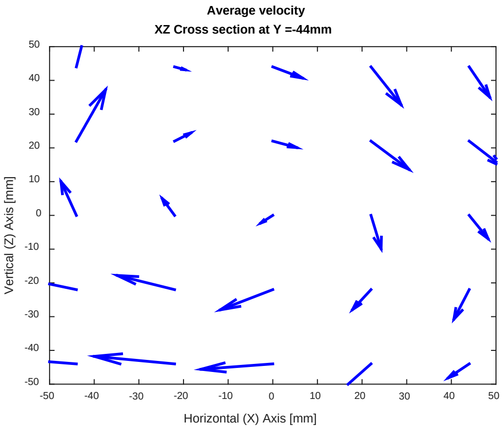
Time-averaged flow field

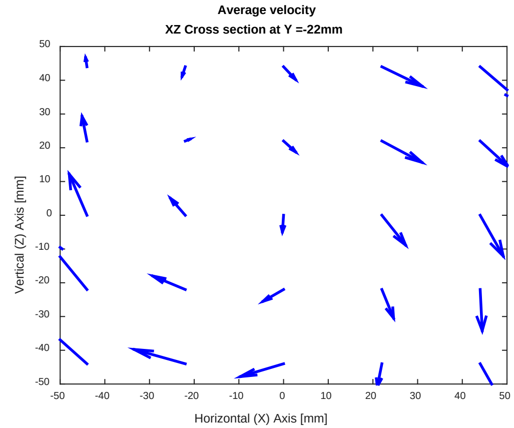


Alpha, LDV

Time-averaged flow field







Impeller “B“
1000 rmp

$$\bar{u} = 0.08$$

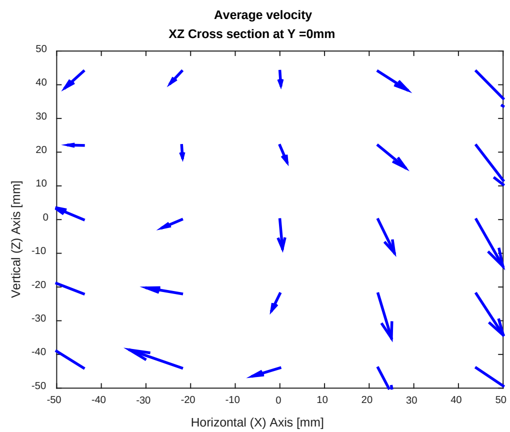
$$\bar{w} = -0.63$$

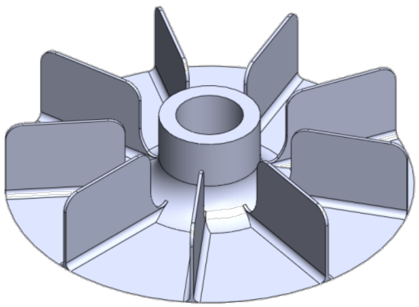
$$u_{rms} = 1.55$$

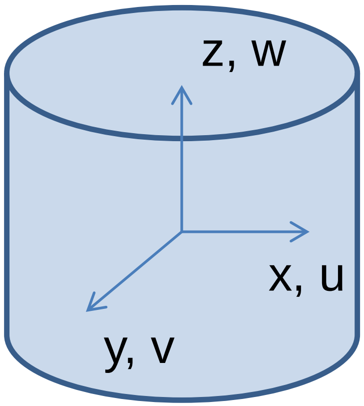
$$w_{rms} = 1.77$$

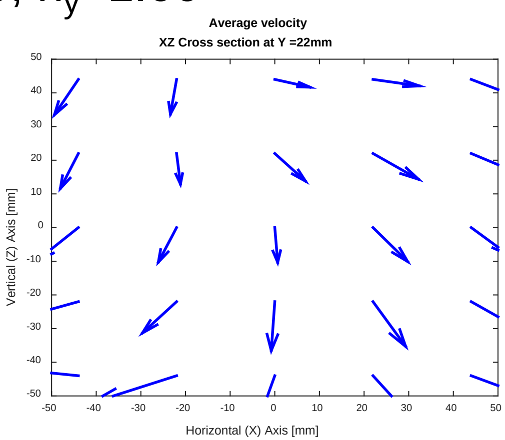
Isotropy = 0.8843

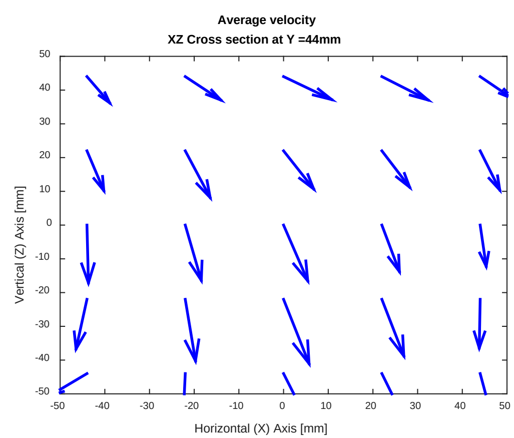
$h_x = 1.00$, $h_y = 1.00$

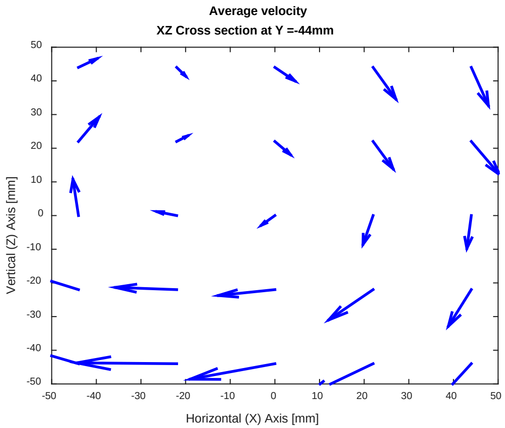


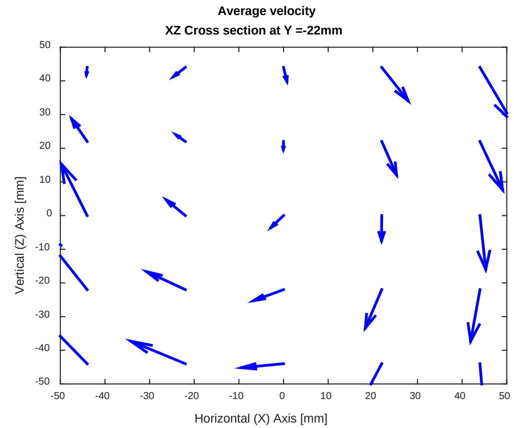










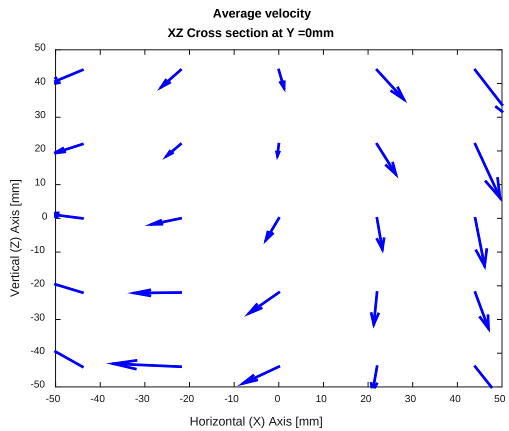


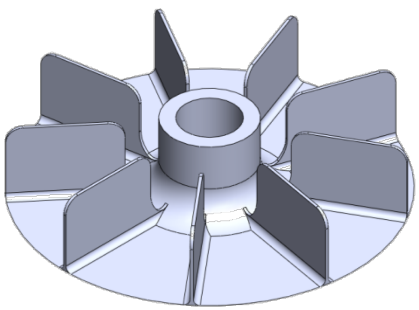
Impeller “B“ 2000 rmp

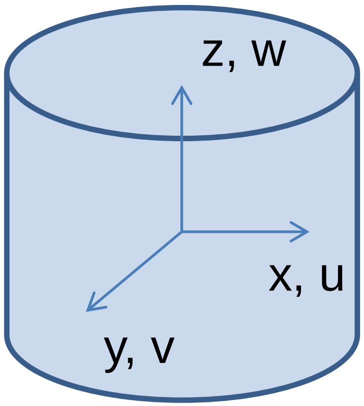
$$\bar{u} = -0.41$$
$$\bar{w} = -0.94$$
$$u_{rms} = 3.11$$
$$w_{rms} = 3.62$$

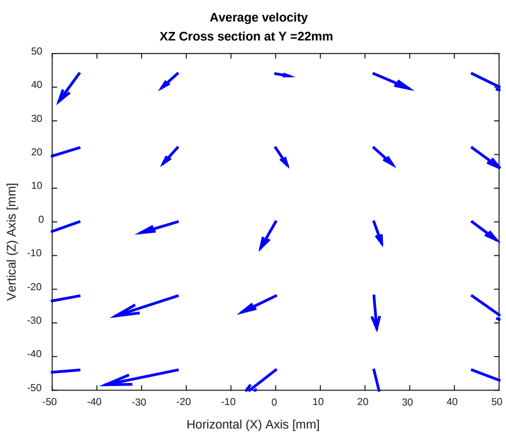
Isotropy = 0.8619

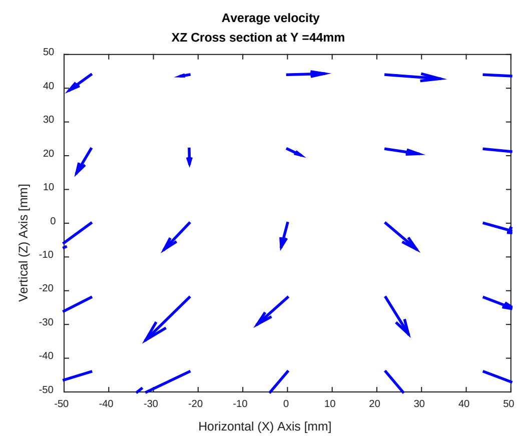
$h_x = 1.02$, h_y=1.01











Power consumption

The load was too great for some impellers