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Flame instability of ammonia aerosol combustion: numerical simulations from astrophysics to industry

A project funded under the “STFC Horizons Programme: investigating solutions for net zero”

Chris Wareing

Collaborators:
Sven Van Loo (PI), Junfeng Yang

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Outline:

- Introduction: net zero fuels
- Numerical model
- Validation through experiments
- Conclusions

Moving towards net zero

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The UK government is committed to reducing the UK's net emissions of greenhouse gases to zero by 2050.

How can research help?

- through driving innovation in renewable energy.
- by creating new technologies to remove greenhouse gases from the atmosphere.

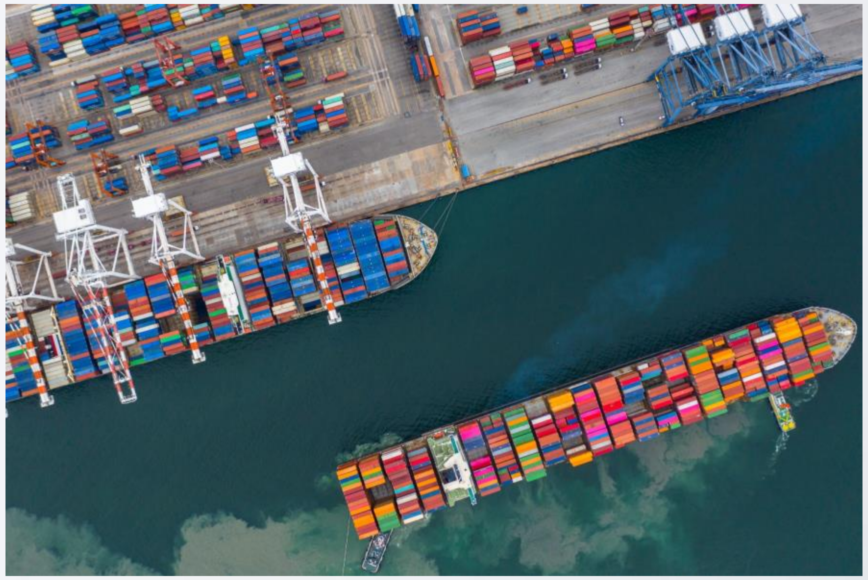
Ammonia - as alternative fuel for engine and gas turbines

Pros:

- Easy to produce from renewable sources of Nitrogen and Hydrogen.
- High energy density (382.6 kJ/mol compared to 286 kJ/mol for hydrogen).
- Only small changes in production, transport and distribution facilities needed.

Cons:

- Production of NOx emissions
- Low reactivity causing unreliable ignition and unstable combustion



Improving combustion

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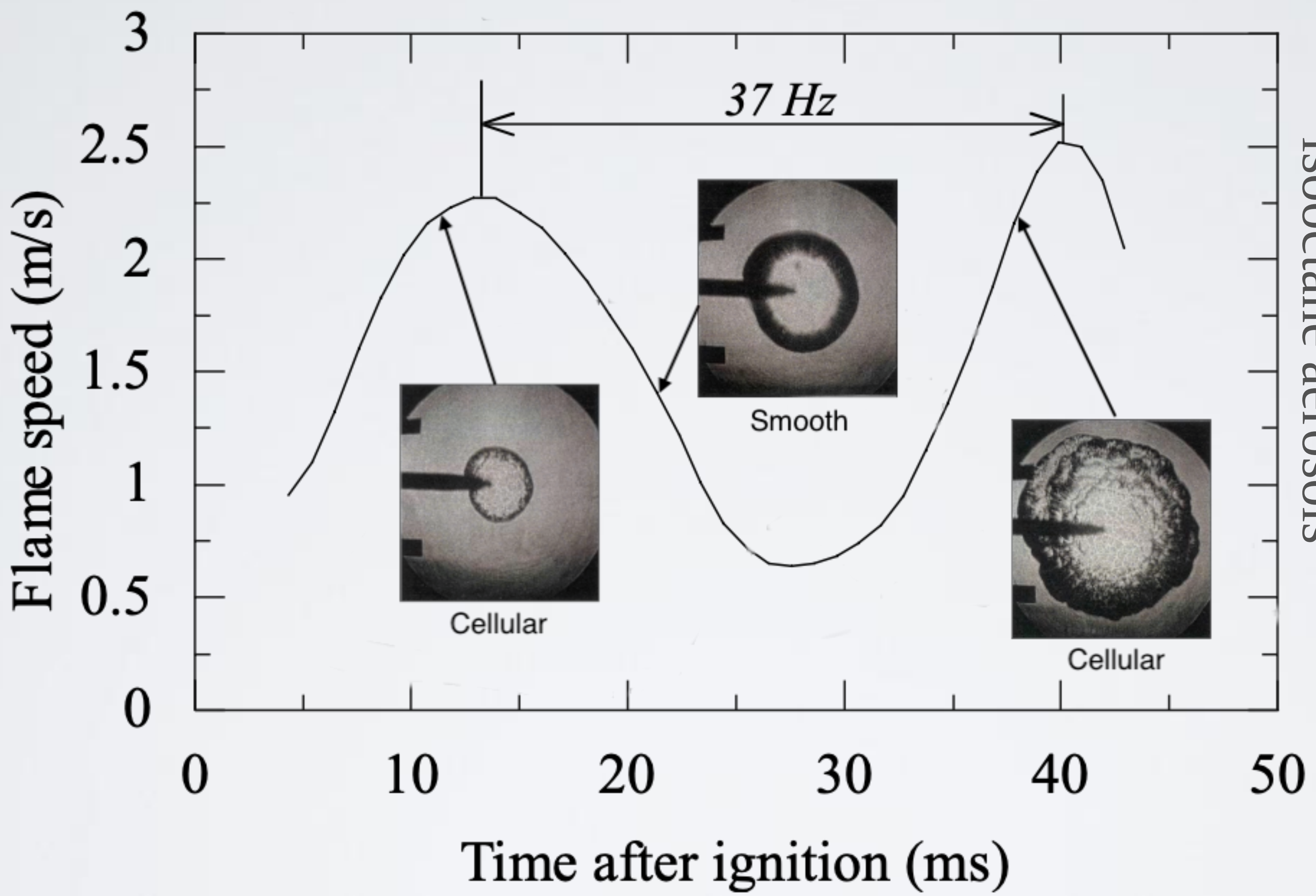
Combustion of aerosol clouds (i.e. clouds of fuel droplets) shows a periodic enhancement of flame propagation speed (at least for hydrocarbon fuels).



isooctane aerosols

The flame acceleration/deceleration process is not fully understood, and it is not known whether the same applies with ammonia.

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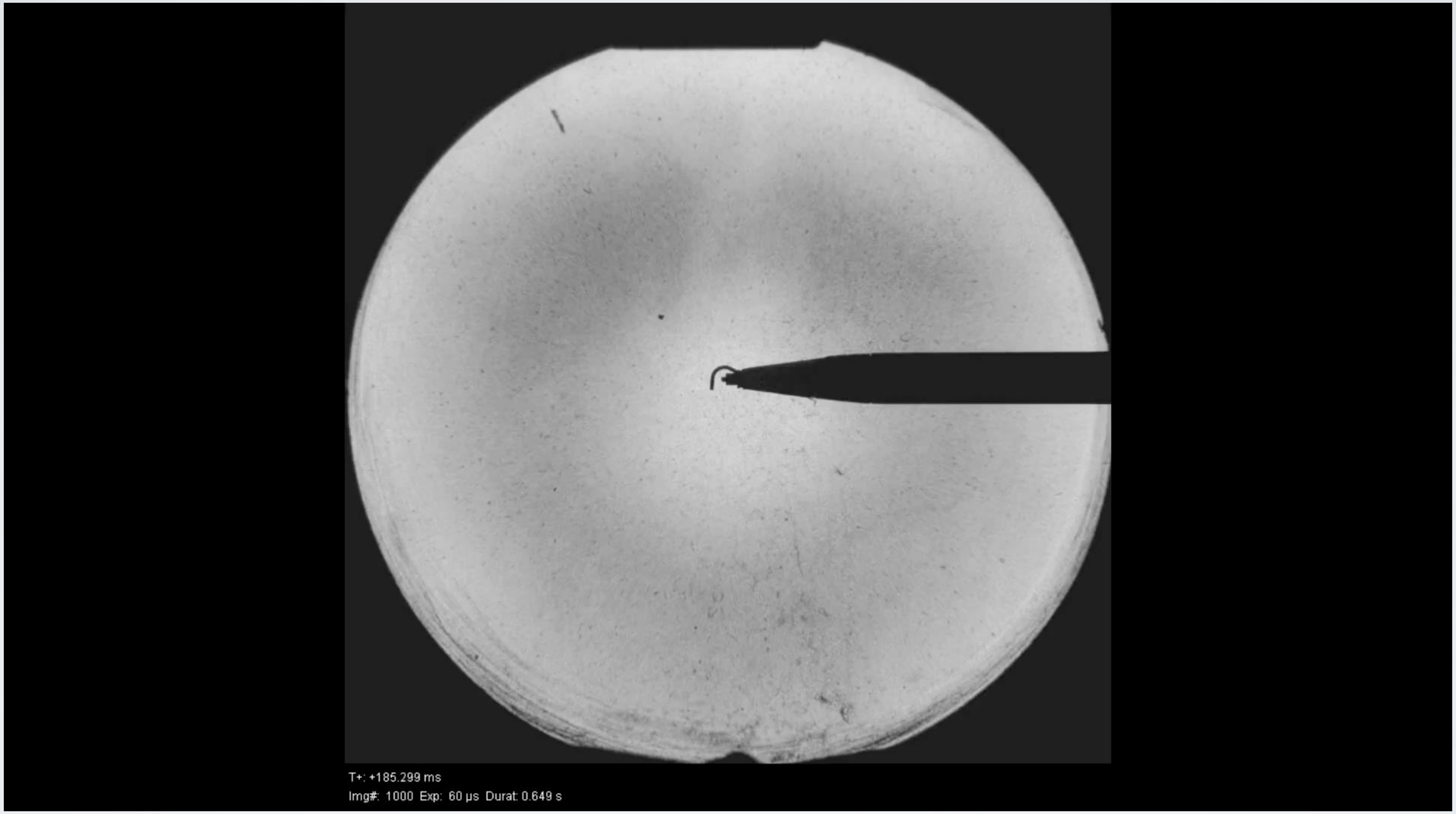

isooctane aerosols

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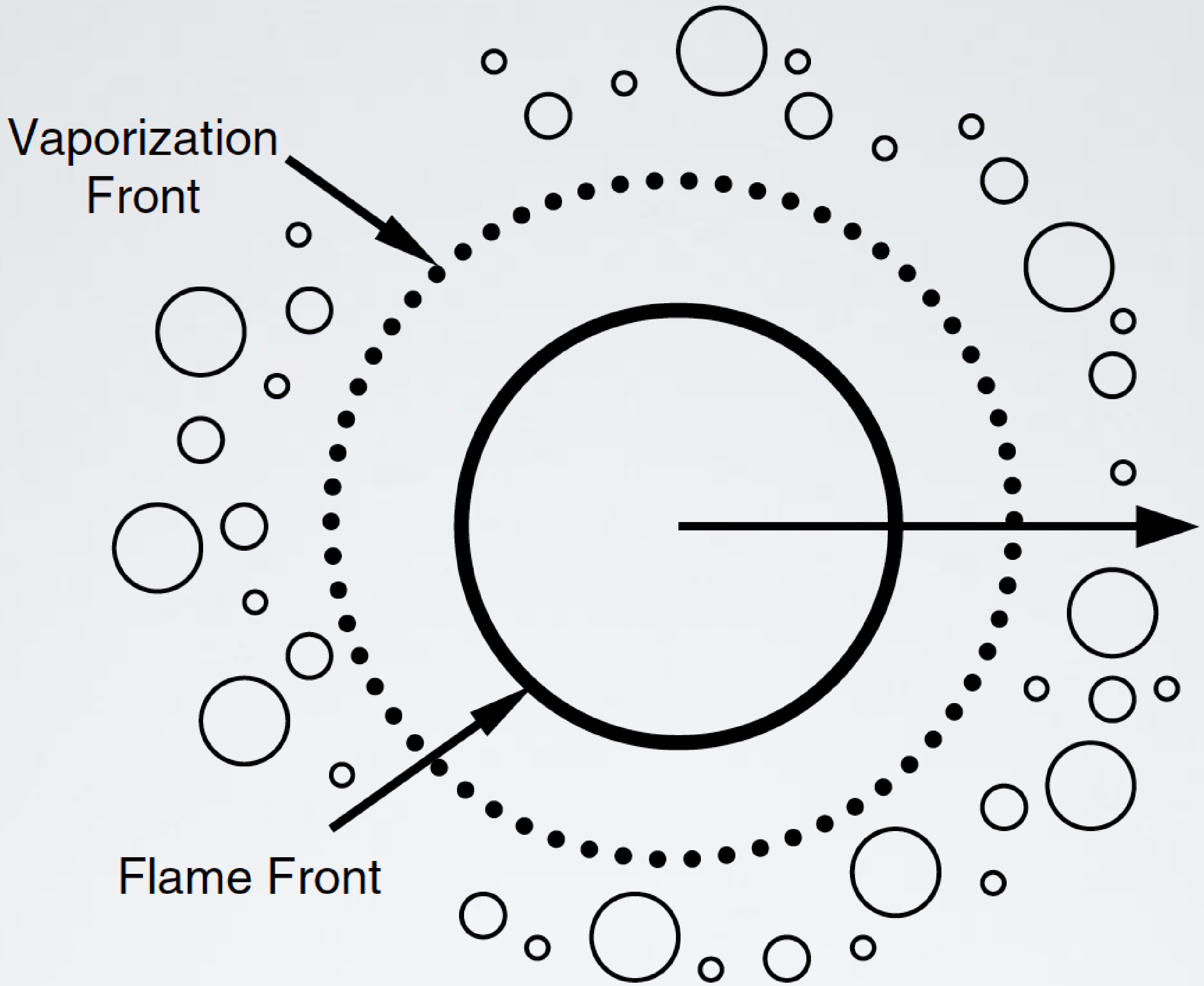
Physical model needs to describe:



- Multi-phase medium: liquid droplets, hot gaseous flame
- Multi-scales: droplet size 10μm, flame thickness 1mm, flame size 10cm
- Multiphysics: droplet evaporation and flame propagation.

Applying tools from astrophysics

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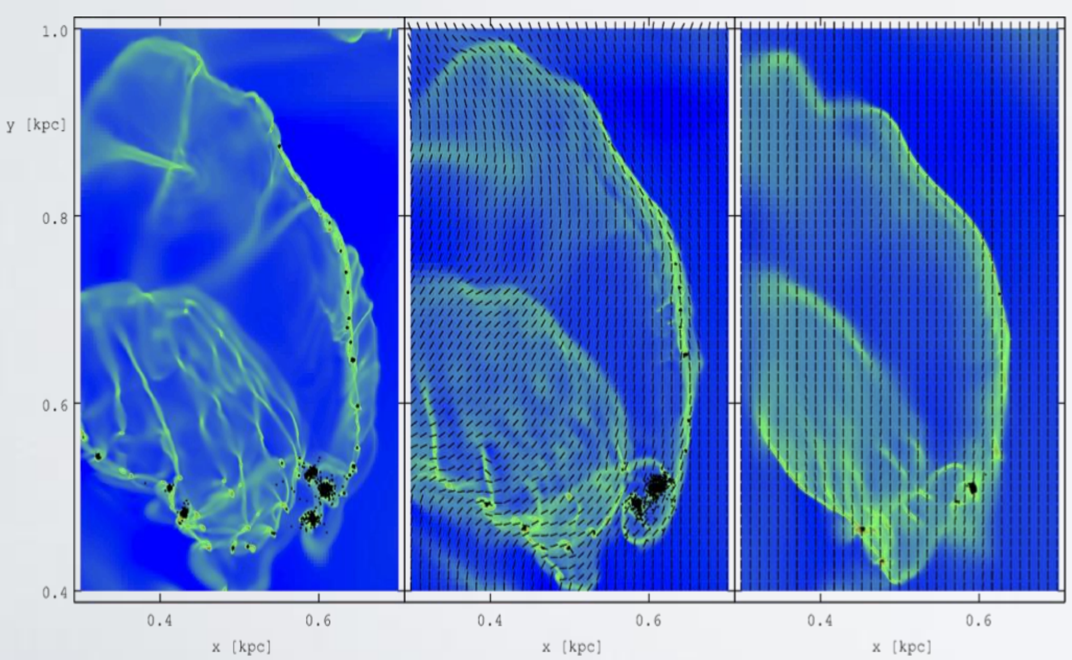
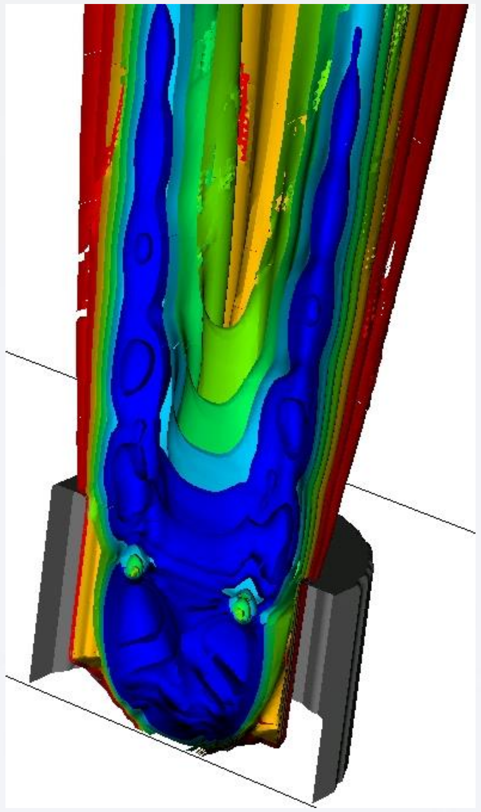
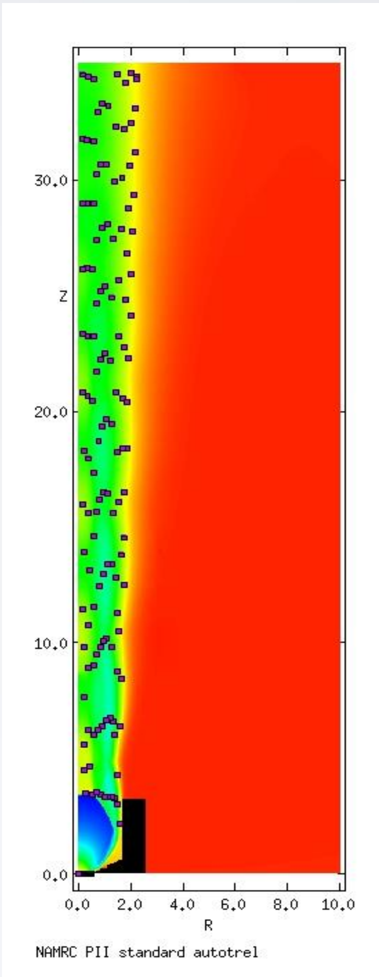
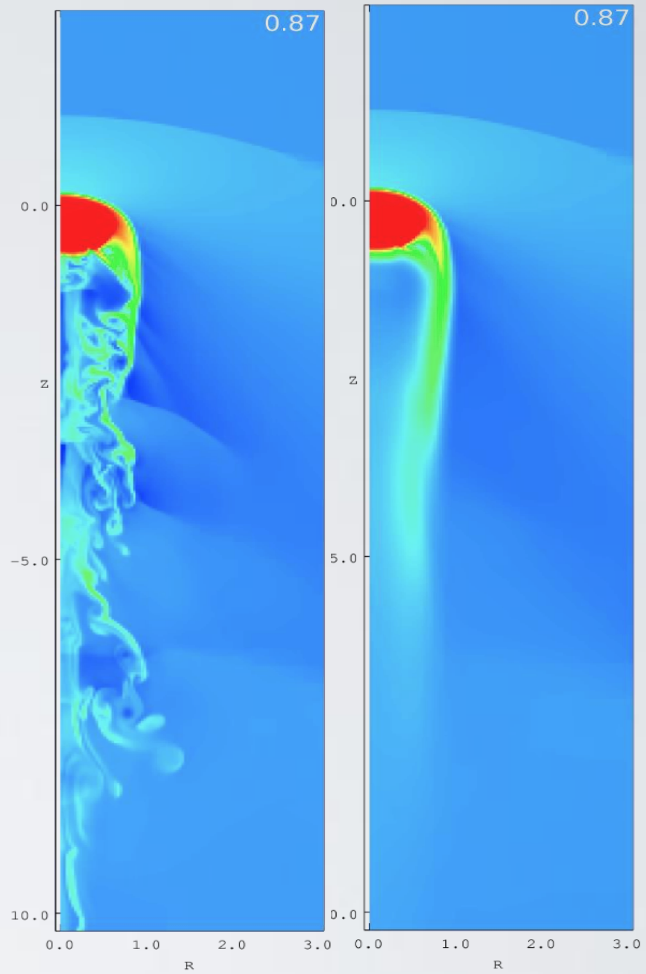
The numerical astrophysics code (MG) has included the techniques we need previously:

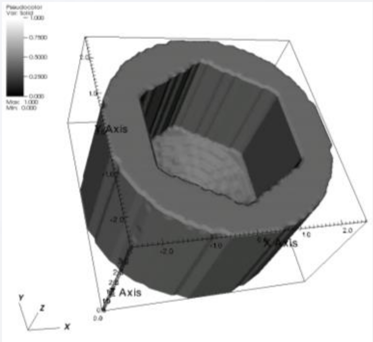
1. Adaptive-mesh refinement to cover large range of scales.
2. Advection-diffusion equation to model combustion.
3. Lagrangian particles for the droplets
4. Subgrid turbulence model
5. Dynamical drag relation
6. Empirical thermodynamic evaporation

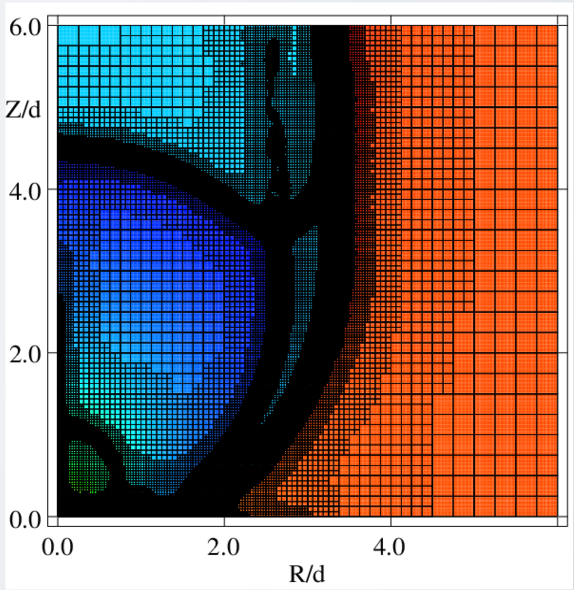












Impact of MG in industrial applications

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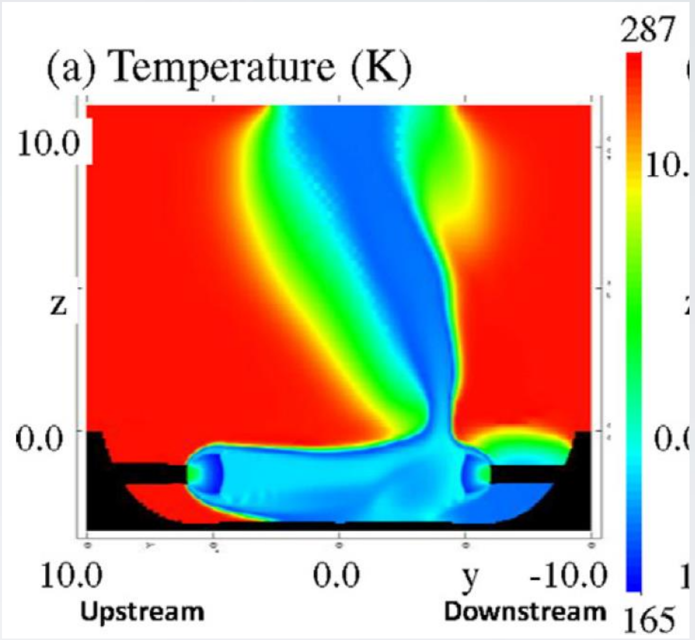
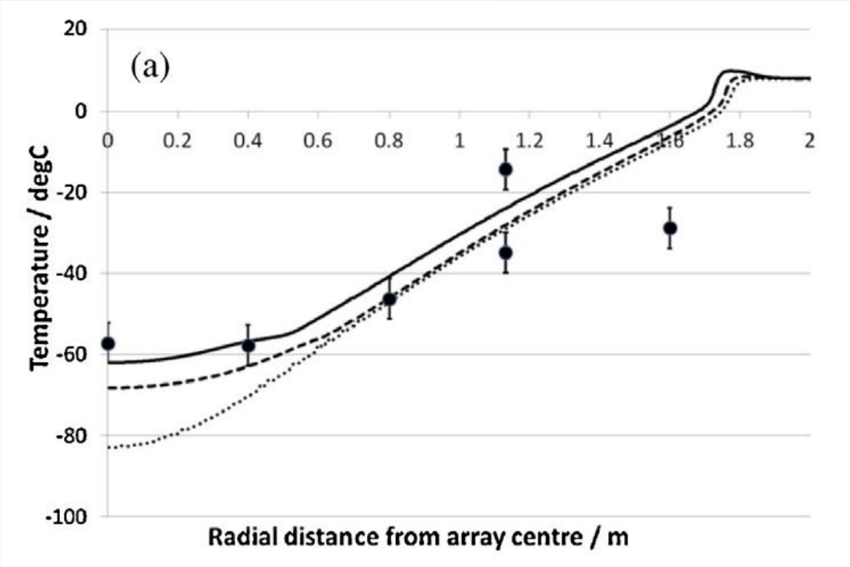
- Carbon capture and storage; simulation of high pressure, dense phase, CO_2 pipelines

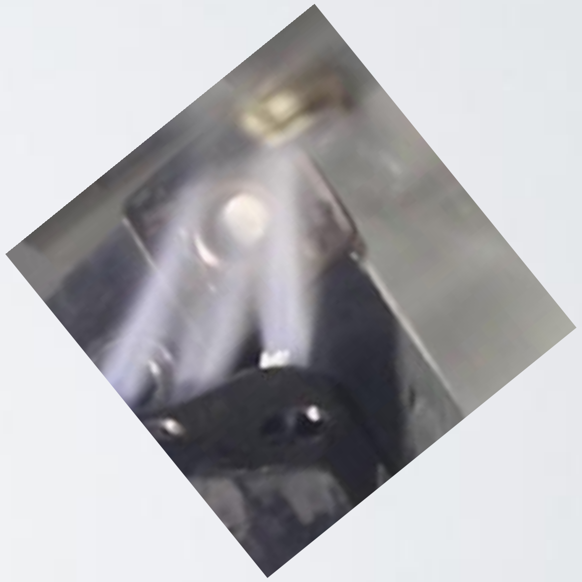
- Cryogenic machining with CO_2

- Explosives modelling for control of chemical processes

- National Grid, British Gas, HSE, HSL, BOC, DNV GL, Seco, Forgemasters, DNV GL, AWE, Bondalti, INNOVNANO







Impact of people

- Knowledge and skills transfer: MScs, PhDs, Post-Docs.
- Of the three projects above, one came about through job destination of MSc.

Thermodynamics

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Combustion model according to Catlin et al. 1995

- Combustion uses progress variable with c= 1 if fuel is burnt and c=0 when unburnt

$$\frac{\partial}{\partial t}(\rho c) + \frac{\partial}{\partial x}(v_x c) = \frac{\partial}{\partial x}\left(\rho \nu_c \frac{\partial c}{\partial x}\right) + \rho S$$

and the reaction included as: $S = Rc^4(1-c)\left(\frac{\rho_u}{\rho_b}\right)^2.$

- Some modification in total energy to reflect energy release

$$\frac{\partial}{\partial t}(\rho e_T) + \frac{\partial}{\partial x}(v_x(\rho e_T + p)) = \frac{\partial}{\partial x}\left(\rho \nu_e \frac{\partial T}{\partial x}\right) + \rho S q$$

with: $q = \left(\frac{P_0}{\rho_u}\right)\left(\frac{\rho_u}{\rho_b} - 1\right)\frac{\gamma}{\gamma - 1}$

Particle evolution model

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- Evolution of particles:

$$\frac{\mathrm{d}\mathbf{v}_p}{\mathrm{d}t} = -\frac{1}{\tau_d}(\mathbf{v}_p - \mathbf{v}_f) + \left(1 - \frac{\rho_f}{\rho_p}\right)\mathbf{g} + \frac{3}{r_p}(\mathbf{v}_f - \mathbf{v}_p)\frac{\mathrm{d}r_p}{\mathrm{d}t}.$$

- Viscous drag in low Reynolds regime accounted for by relaxation time:

$$\tau_d = \frac{2}{9}\frac{\rho_p r_p^2}{\mu}.$$

- Particle evaporation models:

1. Simple temperature difference model (Greenberg 2003):

$$\frac{dm_p}{dt} = \Lambda \kappa e^{\kappa(T - T_v)}$$

3. More complex thermodynamics:

$$\frac{\mathrm{d}m_p}{\mathrm{d}t} = 4\pi\kappa r_p \frac{RT_\infty^2}{L^2 w_v}\frac{[p_\infty - p_s(T_\infty)]}{p_s(T_\infty)}.$$

Current progress

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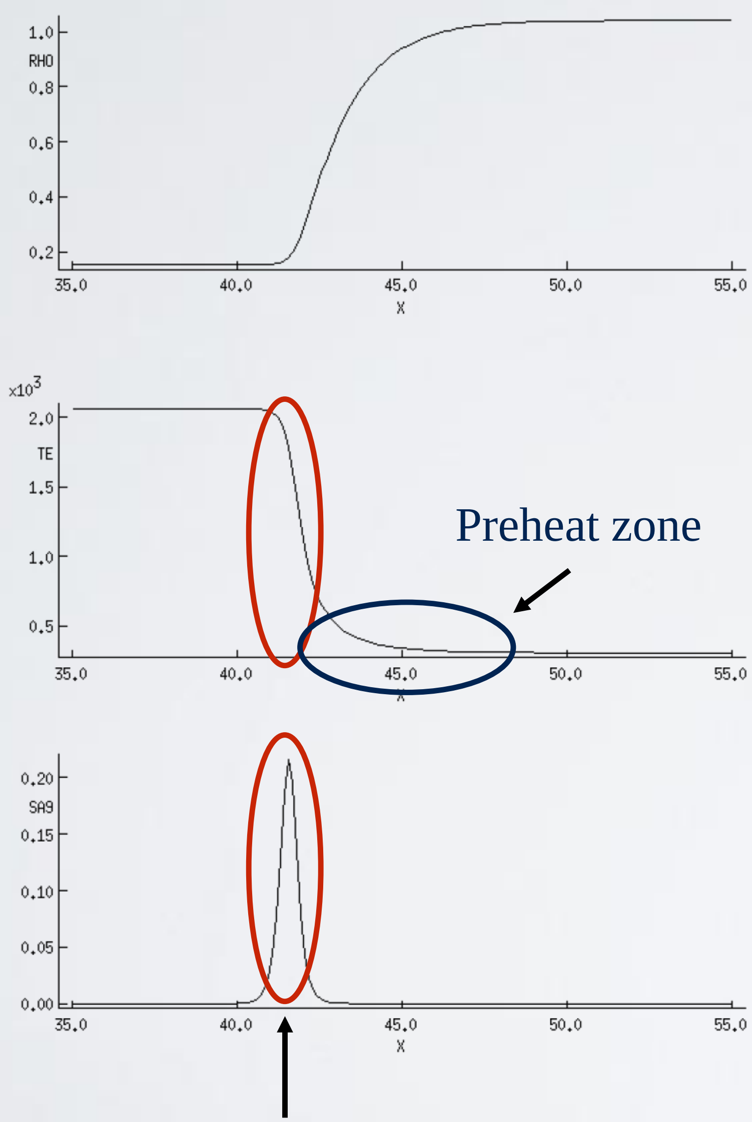
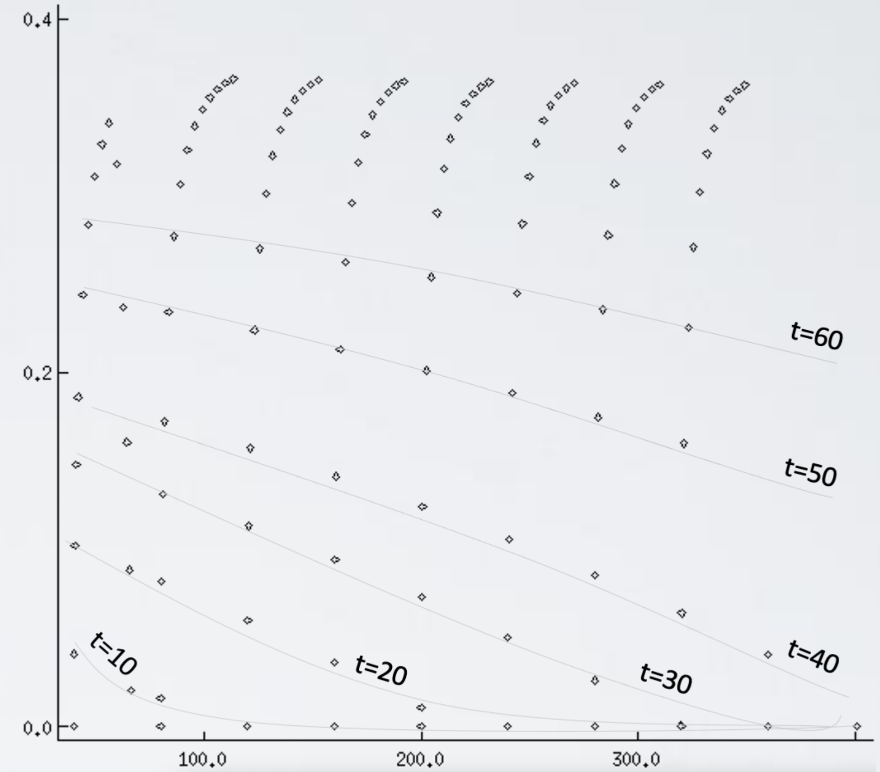
Testing phase of the numerical code: combustion and droplet physics

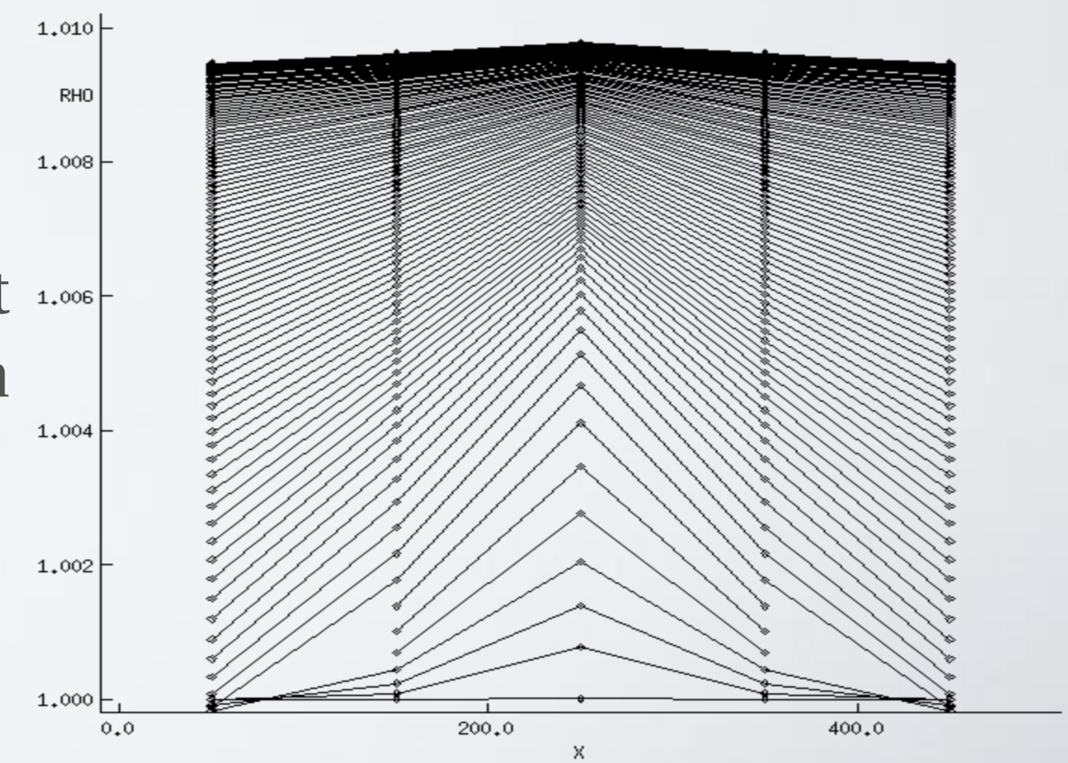
Flame structure





Droplet drag

Droplet evaporation



Experimental work

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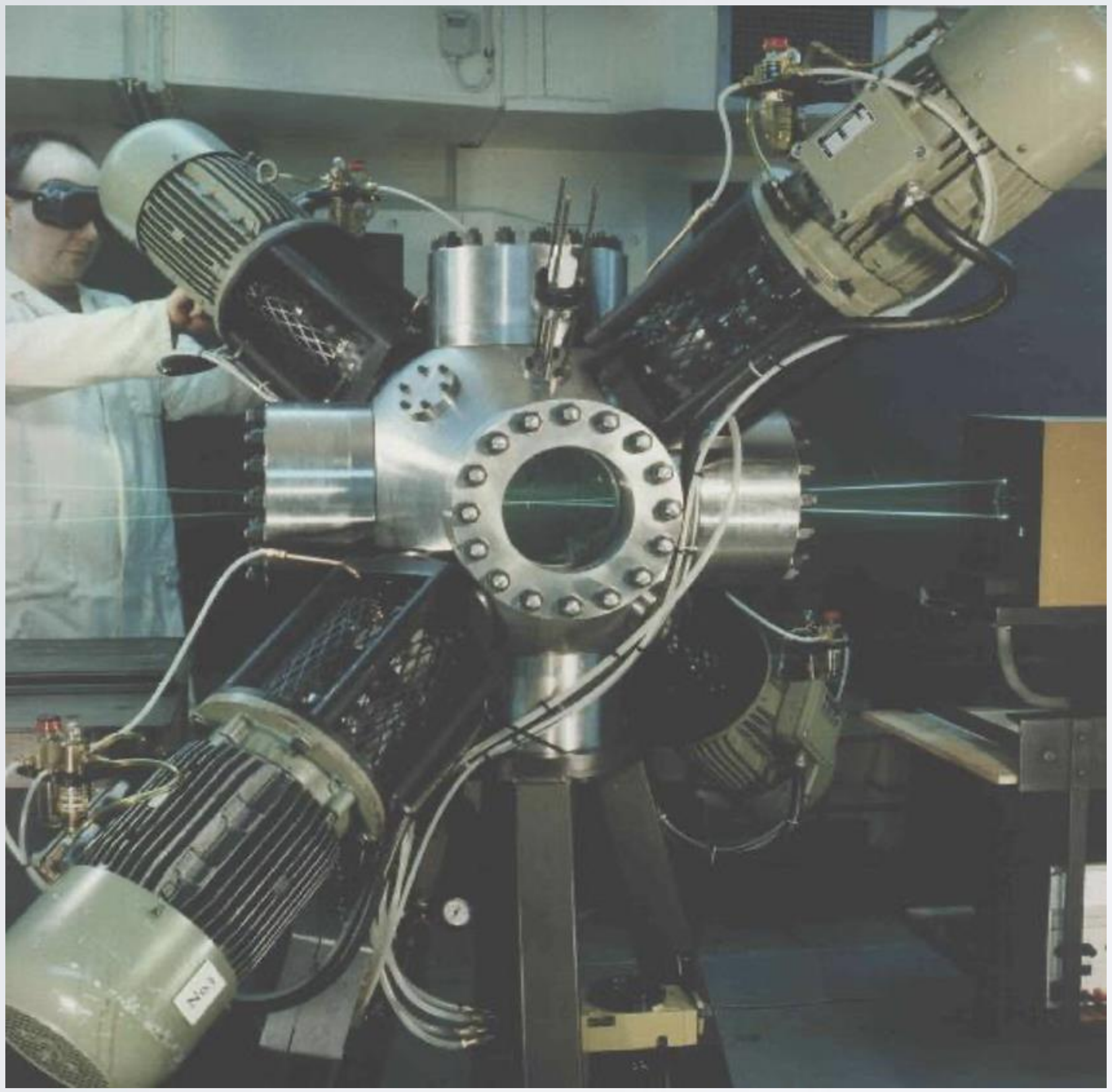
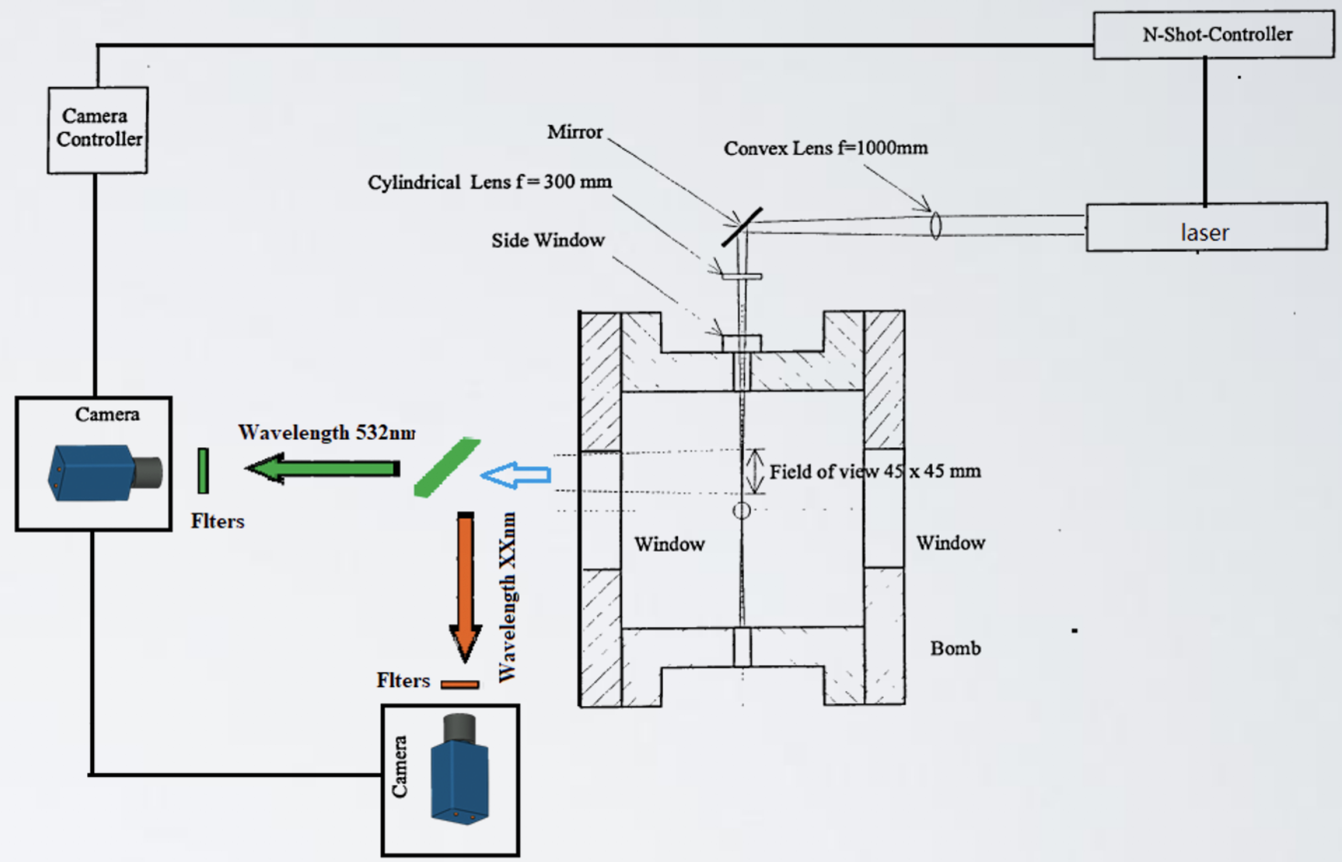
Isooctane experimental data available for validation



Leeds MKII fan-stirred bomb (Bradley lab)



Schematic of the high-speed two-color PIV

Experimental work

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Initial condition from experimental measurement…

Table 1
Measurements with experimental conditions and computed D and R (r_f = 48 mm) for: *i*-octane/air.

ϕ	ϕ_l	P (MPa)	T_u (K)	T_b (K)	d_0 (μm)	$n \times 10^9$ (m^{-3})	ρ_{uo} (kg/m^3)	ρ_b (kg/m^3)	$\bar{\rho}_{uT}$ (kg/m^3)	$\frac{\rho_{uo}}{\rho_b}$	$\frac{\bar{\rho}_{uT}}{\rho_{uo}}$	D	R^2	u_e/u_r (B = 1)
0.8	0	0.120	276	2038	0	0	1.557	0.201	0.410	7.734	–	–	–	–
0.8	0.001	0.121	271	2034	5	1.7	1.599	0.203	0.414	7.866	0.259	0.259	0.975	1.052
0.8	0.229	0.093	263	2022	20	6.4	1.286	0.157	0.318	8.166	0.247	0.264	0.971	1.064
0.9	0.000	0.097	279	2177	0	0	1.249	0.152	0.330	8.240	–	–	–	–
0.9	0.004	0.093	278	2176	5	7.2	1.202	0.145	0.317	8.267	0.263	0.264	0.976	1.054
0.9	0.118	0.097	277	2174	14	9.5	1.268	0.152	0.330	8.345	0.260	0.269	0.977	1.053
0.9	0.243	0.094	265	2164	20	6.8	1.295	0.148	0.320	8.750	0.247	0.264	0.976	1.055
1.0	0	0.097	278	2265	0	0	1.258	0.145	0.328	8.700	–	–	–	–
1.0	0.004	0.095	277	2264	5	7.2	1.237	0.142	0.321	8.729	0.259	0.260	0.979	1.048
1.0	0.035	0.089	272	2259	10	7.2	1.183	0.133	0.301	8.888	0.254	0.257	0.978	1.051
1.0	0.127	0.099	278	2263	14	10.0	1.294	0.148	0.334	8.758	0.258	0.267	0.980	1.049
1.0	0.215	0.099	273	2259	18	8.4	1.326	0.148	0.334	8.953	0.252	0.267	0.979	1.051
1.0	0.244	0.096	268	2255	20	6.9	1.313	0.144	0.324	9.122	0.247	0.264	0.978	1.053
1.1	0	0.097	279	2265	0	0	1.258	0.143	0.323	8.827	–	–	–	–
1.1	0.125	0.102	278	2263	14	10.0	1.338	0.150	0.340	8.915	0.254	0.263	0.983	1.042
1.1	0.337	0.098	270	2254	20	9.6	1.343	0.145	0.326	9.271	0.243	0.266	0.981	1.047
1.2	0	0.100	280	2203	0	0	1.297	0.148	0.327	8.743	–	–	–	–
1.2	0.004	0.100	280	2202	5	7.6	1.297	0.148	0.327	8.745	0.252	0.252	0.984	1.037
1.2	0.036	0.093	275	2198	10	7.5	1.231	0.138	0.304	8.904	0.249	0.249	0.983	1.037
1.2	0.128	0.105	279	2200	14	11.0	1.378	0.156	0.343	8.834	0.249	0.258	0.985	1.034
1.2	0.293	0.103	270	2191	18	12.0	1.412	0.154	0.337	9.184	0.238	0.259	0.985	1.036

Bradley et al. 2014, Combustion and Flame, 161, 1620-1632

Full thermodynamic properties from software

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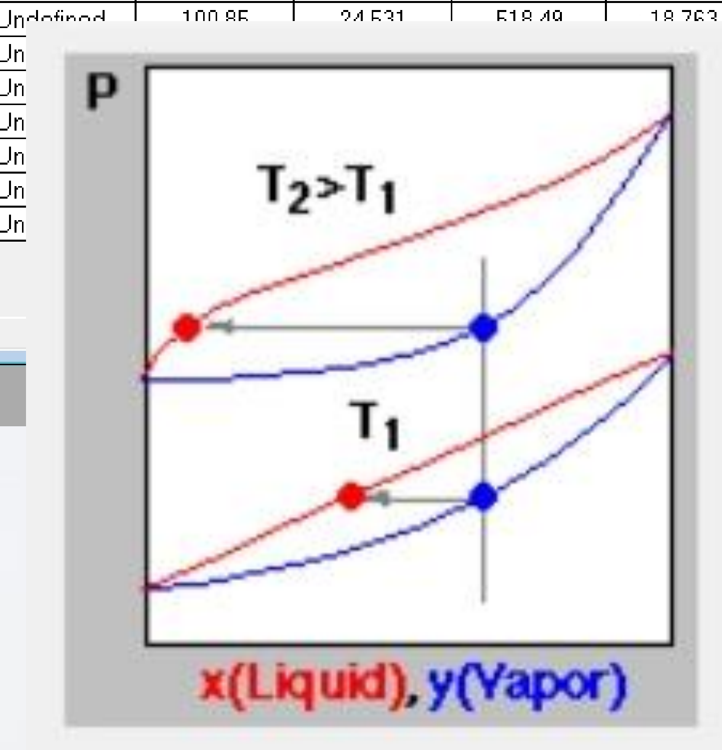
Vapor at dew point with coexisting liquid from thermodynamic software e.g. REFPROP10

REFPROP - NIST Reference Fluid Properties (DLL version 10.0)

File Edit Options Substance Calculate Plot Window Help Cautions

3: Isooctane/Nitrogen/Oxygen: Dew Point. T=250.0 to 290.0 K (1.6522/20.653/77.695)

	Temperature (K)	Pressure (MPa)	Liquid Phase Density (g/cm³)	Vapor Phase Density (g/cm³)	Liquid Phase Cp (J/g-K)	Vapor Phase Cp (J/g-K)	Liquid Phase Cp0 (J/g-K)	Vapor Phase Cp0 (J/g-K)	Liquid Phase Cp/Cv	Vapor Phase Cp/Cv	Heat of Vapor. (J/g)	Liquid Phase Therm. Cond. (mW/m-K)	Vapor Phase Therm. Cond. (mW/m-K)	Liquid Phase Viscosity (μPa-s)	Vapor Phase Viscosity (μPa-s)	Liquid Phase Kin. Viscosity (cm²/s)
1	250.00	0.073214	0.73429	0.0011088	1.8798	0.94847	1.3781	0.94661	1.2766	1.3896	Undefined	109.05	22.137	833.06	17.128	0.011345
2	252.00	0.084169	0.73290	0.0012647	1.8870	0.94899	1.3865	0.94689	1.2756	1.3897	Undefined	108.45	22.304	802.51	17.244	0.010950
3	254.00	0.096512	0.73151	0.0014390	1.8943	0.94953	1.3949	0.94717	1.2746	1.3899	Undefined	107.86	22.471	773.56	17.360	0.010575
4	256.00	0.11039	0.73012	0.0016332	1.9015	0.95010	1.4034	0.94746	1.2736	1.3900	Undefined	107.26	22.638	746.11	17.476	0.010219
5	258.00	0.12595	0.72872	0.0018493	1.9088	0.95071	1.4118	0.94775	1.2727	1.3902	Undefined	106.67	22.806	720.05	17.592	0.0098810
6	260.00	0.14337	0.72732	0.0020892	1.9161	0.95136	1.4202	0.94805	1.2717	1.3904	Undefined	106.08	22.975	695.29	17.708	0.0095596
7	262.00	0.16284	0.72591	0.0023551	1.9235	0.95204	1.4285	0.94835	1.2708	1.3907	Undefined	105.49	23.144	671.73	17.824	0.0092536
8	264.00	0.18454	0.72450	0.0026493	1.9308	0.95276	1.4369	0.94865	1.2699	1.3910	Undefined	104.90	23.314	649.31	17.941	0.0089621
9	266.00	0.20871	0.72309	0.0029742	1.9382	0.95353	1.4452	0.94897	1.2690	1.3913	Undefined	104.32	23.485	627.95	18.057	0.0086842
10	268.00	0.23557	0.72167	0.0033326	1.9456	0.95434	1.4536	0.94928	1.2682	1.3917	Undefined	103.73	23.656	607.57	18.174	0.0084189
11	270.00	0.26537	0.72025	0.0037272	1.9531	0.95520	1.4619	0.94960	1.2674	1.3922	Undefined	103.15	23.829	588.12	18.291	0.0081655
12	272.00	0.29840	0.71882	0.0041613	1.9605	0.95611	1.4701	0.94993	1.2666	1.3926	Undefined	102.57	24.002	569.54	18.408	0.0079232
13	274.00	0.33496	0.71739	0.0046381	1.9680	0.95709	1.4784	0.95027	1.2658	1.3932	Undefined	101.99	24.177	551.78	18.526	0.0076914
14	276.00	0.37537	0.71596	0.0051612	1.9755	0.95812	1.4866	0.95060	1.2651	1.3938	Undefined	101.42	24.353	534.78	18.644	0.0074694
15	278.00	0.41999	0.71452	0.0057347	1.9830	0.95921	1.4948	0.95095	1.2643	1.3944	Undefined	100.85	24.531	518.49	18.763	0.0072566
16	280.00	0.46921	0.71307	0.0063629	1.9905	0.96038	1.5029	0.95130	1.2636	1.3952	Un	[illegible]	[illegible]	[illegible]	[illegible]	0.0070524
17	282.00	0.52346	0.71162	0.0070503	1.9980	0.96161	1.5111	0.95165	1.2630	1.3960	Un	[illegible]	[illegible]	[illegible]	[illegible]	0.0068563
18	284.00	0.58322	0.71016	0.0078023	2.0055	0.96293	1.5191	0.95201	1.2624	1.3969	Un	[illegible]	[illegible]	[illegible]	[illegible]	0.0066679
19	286.00	0.64898	0.70870	0.0086244	2.0130	0.96433	1.5272	0.95238	1.2618	1.3978	Un	[illegible]	[illegible]	[illegible]	[illegible]	0.0064866
20	288.00	0.72134	0.70724	0.0095230	2.0206	0.96582	1.5351	0.95275	1.2612	1.3989	Un	[illegible]	[illegible]	[illegible]	[illegible]	0.0063121
21	290.00	0.80100	0.70577	0.010505	2.0281	0.96741	1.5431	0.95313	1.2607	1.4001	Un	[illegible]	[illegible]	[illegible]	[illegible]	0.0061439



We also use GASEQ, CHEMKIN

Iso-octane initial condition

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Vapor – stoichiometric (100% burn) air/isooctane mixture

- 272 K, 0.089 MPa (~0.88 atm.)
- Gamma, C_p/C_v = 1.360
- Unburnt density 1.2067 kg/m^3, burnt density 0.136 kg/m^3
- Specific heat capacity, C_p 248.15 cal/kg/K
- Kinematic viscosity 1.43366x10-5 m^2/s
- Prandtl number, Pr 0.825576

Derive the necessary remaining properties – dynamic viscosity, thermal conductivity…

Particles

- 272 K, at saturation pressure of 0.095603 MPa
- density of 0.71225 kg/m^3
- Latent heat of vaporisation 484.66 J/g

Promising preliminary results

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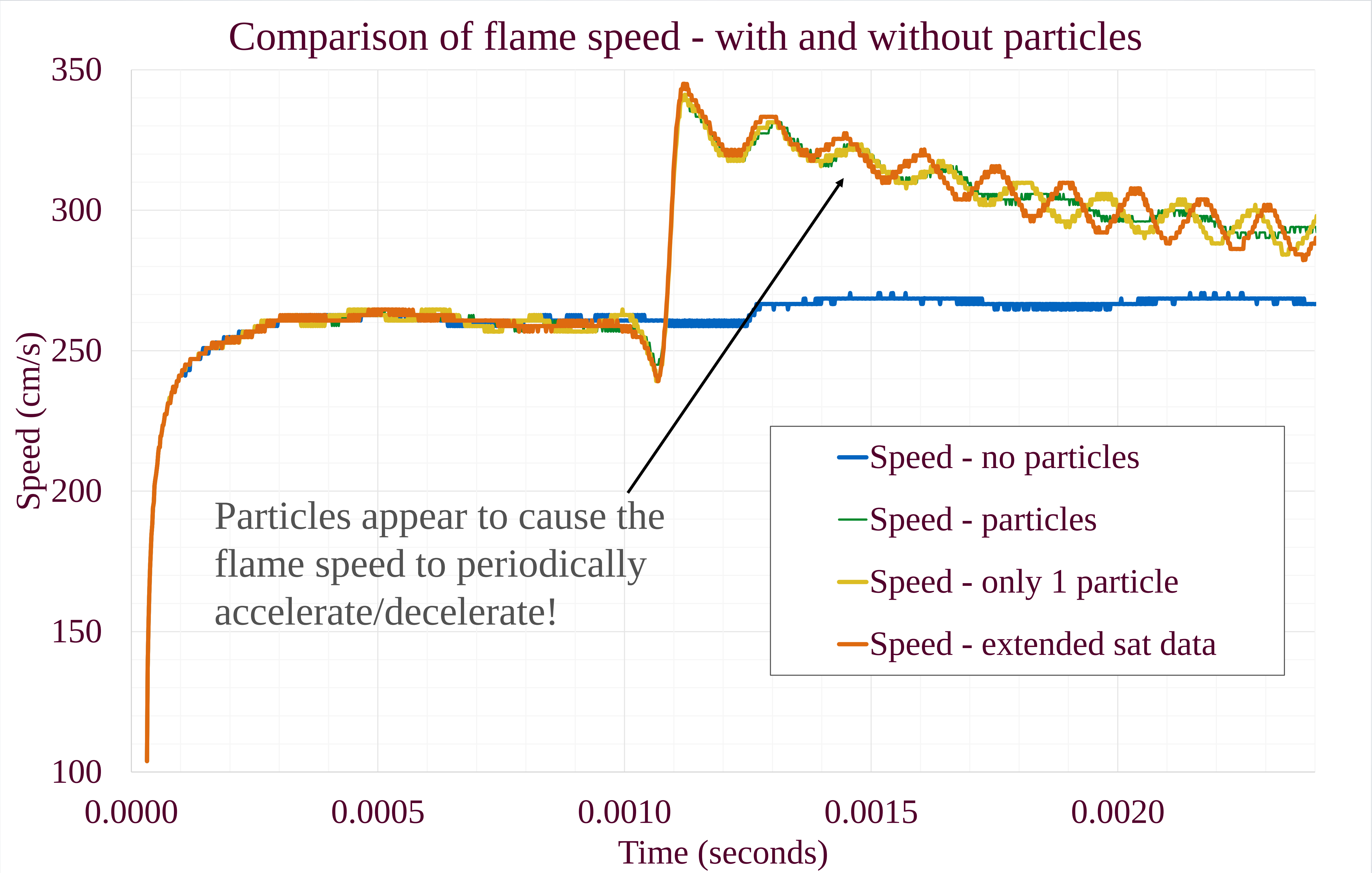

Future Work

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- Application to ammonia
- Validation through ammonia experimental data
- Inclusion of chemistry to deal with NOx emission

Conclusions

- Use of existing techniques applied to a ‘new’ field: thinking out-of-the-box
- Contribution to fundamental research towards net-zero.
- Deliver numerical code that can be used to model more realistic situations