

SATELLITE LAUNCHERS

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SPACE LAUNCHERS TO ORBIT PAYLOAD

► **ORBITING = V + height** [$V = f(h)$, $h \sim 100 \text{ km to } 36,000 \text{ km}$]

► Energy in orbit, per unit mass: $E = 1/2 V^2 + gh$

e.g.: at height $\sim 400 \text{ km}$, orbital $V \sim 8.2 \text{ km/s}$ and $E \sim 3.2 \times 10^7 + 4 \times 10^6 \text{ J/kg}$

Burning 1 kg gasoline + air $O_2 \rightarrow 4.4 \times 10^6 \text{ J}$

the ideal energy to orbit payload using external air is not much...

LAUNCHERS: REALITY CHECK

To accelerate (V) and lift (h) P/L to orbit: Newton's 3rd Law → **thrust**

- ▶ **Thrust:** burn propellants and expand exhaust in a nozzle at high V_e from either a 1. **rocket** or 2. an airbreathing engine
- ▶ 1. **Rocket** engines burn fuel with onboard oxidizer:
 - launcher must be designed to carry oxidizer
 - thrust must accelerate P/L **and** the launcher
 - Propellants: solid, liquid and combinations (hybrid)
- ▶ Rocket **efficiency:** low. V_e is limited by chemistry and thermodynamics
- ▶ Most energy released by burning propellants becomes waste heat (entropy)
Efficiency even worse than that of car engines...

LAUNCHERS: CHEMICAL ROCKETS EFFICIENCY IS LOW

- To accelerate by $\Delta(V)$ a rocket expels **mass** from the nozzle at **$V_e (= I_{sp})$**
 I_{sp} = propellants consumption per unit thrust ~ 2500 to 4600 m/s **at most**

- Hence, from Tsiolkowski's Law:

- $$\Delta(V) = I_{sp} \ln(W_{initial} / W_{final}) \quad \text{or}$$

$$W_{fin} = W_{init} \exp(-\Delta(V) / I_{sp})$$

- But: to reach LEO, $\Delta(V)$ must be at least ~ 8000 m/s...

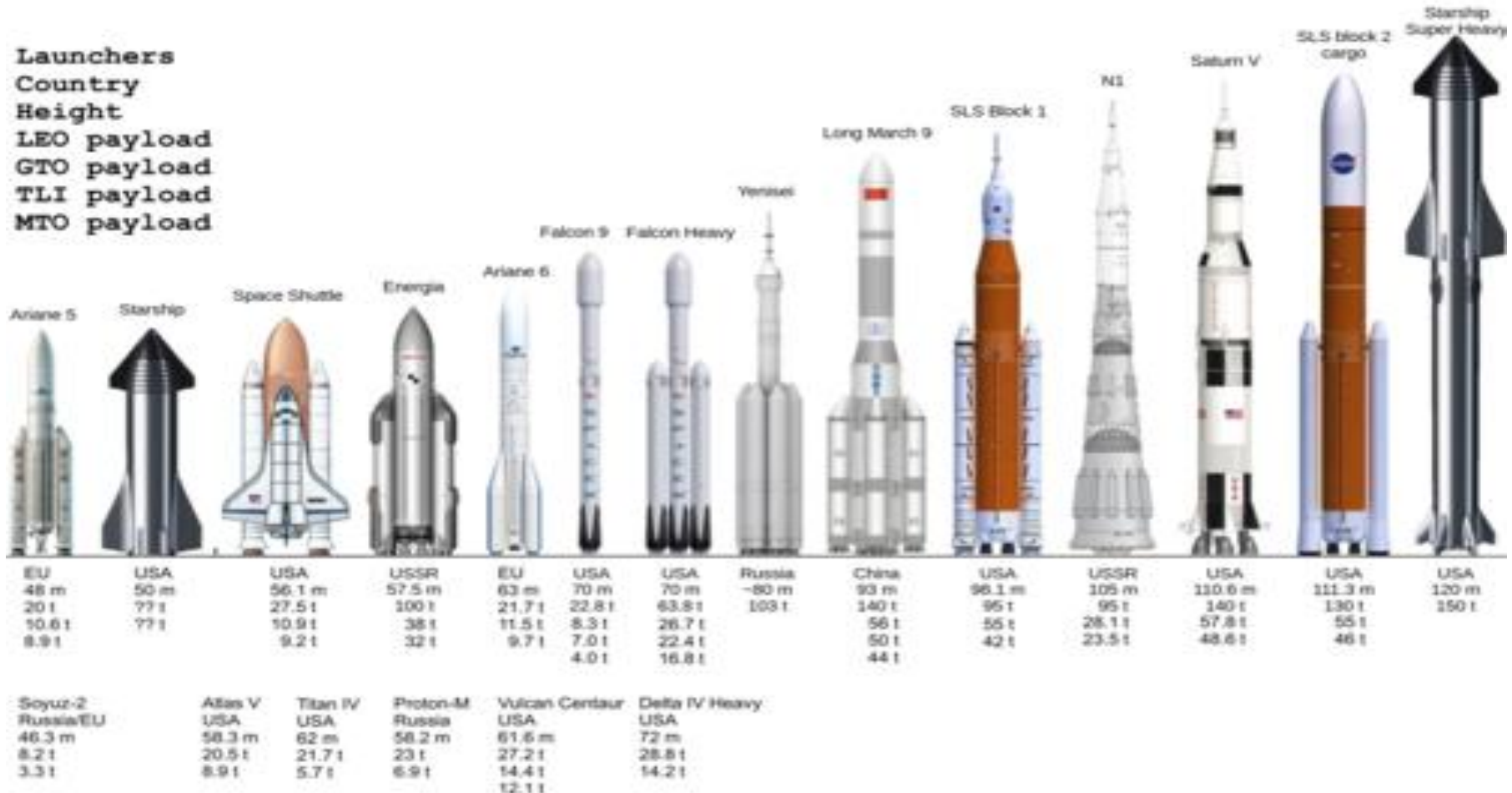
Thus: **$\Delta(V) \gg I_{sp}$** : propellants **mass** to orbit P/L to LEO is huge...
the **W_{fin} / W_{init}** of all rocket launchers is $\sim 1-3$ %

LAUNCHERS: P/L AND MASS

► Launcher mass = P/L + propellants + rocket engine + structure

P/L: ~ 1 to 2×10^5 kg

Total launcher mass : $\sim 10^2$ to 10^3 metric tons



LAUNCHERS: COST

- ▶ Varies with P/L, mission and technology
- ▶ P/L to LEO: ~ 1000 to 20,000 \$/kg
- ▶ P/L to GEO: ~ 25,000 \$/kg
- ▶ rough cost division of orbiting P/L:
 - 1/3 launcher
 - 1/3 ground support
 - 1/3 insurance
- ▶ one Ariane 5 launch: M\$ 100. Ariane 6 *should* be M\$ 115
- ▶ one turbopump: 1 to 3 M\$ for a mid-lift launcher
(‘a rocket launcher is a pair of turbopumps’...)

LAUNCHERS: NEAR TERM PROGRESS

► Rocket technology progress:

- Seals, bearings for cryo turbopumps
- Thermal Protection Systems
- Fuels:
 - LCH₄
 - metal additives for SP (nano-Al, Zr, B...)
 - green fuels (H₂O₂, other)
- Turbopumps
- Structure: composites (CMC, MMC,...)
- Recoverable stages & boosters (SpaceX, iSpace, Hyperbola 3,...)

LAUNCHERS: MID- AND LONG-TERM PROGRESS

► FUELS/OXIDIZER COMBINATIONS

- No magic propellants: LH2, LOX here to stay
- LH2 - H2O2 combinations, LCH4 - LO2
- Low-cost Hybrid Propellants: wax – LO2, wax – H2O2
- propellants replacing hydrazines



► ELECTRIC PROPULSION: • 3rd and 4th stages, maneuvering, verniers...

- Interplanetary missions,
- Deorbiting (zero space debris)

► NUCLEAR PROPULSION: • Thermal, $I_{sp} \sim 10^4$ m/s, large/very large T

- Electric, $I_{sp} \sim 10^6$ to 10^7 m/s, low thrust
- Fusion, large T, high I_{sp}

LAUNCHERS FOR SPACE MISSIONS

- ▶ **TRADING Thrust with Isp:** various combinations, to be tested, e.g.
VASIMR VX-200, $I_{sp} \sim 50,000$ m/s, $T \sim 5$ N
NPT vs. NEP and combinations, to be tested
Fusion: far future
- ▶ **GRAVITY ASSIST:** tested, depends on astrodynamics, slow trajectories: science missions
- ▶ **SPACE HIGHWAYS:** tested once, slow trajectories: cargo app

Antonio Ferri – Impact on SCRJ R&D

- ▶ Ferri's and Fred Billig's work inspired Douglas (later: McDonnell-Douglas, MDD) to work in hypersonic propulsion (see Hallion's paper, AIAA J)
 - MDD designed and built a LH₂-fueled vehicle in late '60s - early '70.
 - Vehicle flew successfully and...
 - was promptly canceled by Bob McNamara after JFK died, as “too destabilizing [the US-SU power balance]”
- ▶ In SU Shchelkin drove Moscow and Novosibirsk teams to explore SC.
 - ITAM work in Novosibirsk (V. Baev, P. Tret'yakov) resulted in a Mach 7 kerosene SCRJ. Mission: to intercept the US Shuttle
 - Also ITAM designed a 27-mm base burning round (fielded)
 - Freishtadt's hypersonic AYAKS concept

Antonio Ferri – SCRJ heritage and current status

- ▶ Major switch in the '90s: to kerosene instead of LH2 (logistics)
- ▶ Russia: classified all SCRJ information after Putin; Granit III evolved to Mach 4.5-5. March 2016 press release by Russian RP describes a Mach 7+ vehicle being prototyped
- ▶ US: R&D and some time-limited testing known (e.g., X-51a); proposals by Aerojet to go to Mach 10 still not funded; work on SCRJ-powered missiles at Raytheon. Very cautious progress after NASP 'failure'
- ▶ China: major player, due to 10-yr R&D at HAI-CARDC & at NPU; flight tested a SCRJ-powered missile in 2010 or 2011
- ▶ South Korea: fielded a RJ-powered anti-IRBM missile; ongoing work toward SCRJ

Antonio Ferri – SCRJ heritage and current status (ctnd)

- ▶ UK: fundamental work in the '70s by Jim Swithenbank clarified turbulent mixing & injection using kerosene. Classified RJ and SCRJ work at Qinetiq. Australia: R&D for Mach 10+ SC for RBCC using 'radical farming' strategy. [Ongoing collaboration among U. Sidney, AU and UK military, and USAF.]
- ▶ India: after solving flame-anchoring issue collaborates with Russia (BrahMo program) to evolve Indian version of Granit II. Plans to USE SC to build RBCC engines
- ▶ France: focus on RDE; successful tests performed. RDE is being applied to a Mach 3.5 AA missile ("Proteus") with longer range than Meteor
- ▶ Norway, Sweden: developed and tested independently Mach 4 - 4.5 RJ-powered antiship (?) missiles.
- ▶ Brazil: SC research, using Nagamatsu's hypersonic WT at RPI, now in Brasilia.

Antonio Ferri – Conclusions

After a protracted R&D period (due in the US by stop-and-go funding), the Ferri's pioneering work spurred worldwide activity now reaching engineering stage.

SCRJ R&D *may* evolve to produce RBCC concepts to power more efficient space launchers

But most applications still military, just as in Ferri's time.

Ferri's vision took more than half century to lose its exotic aura, hampered as it was by rocket industry hostility, tinkering and inflated promises, and is now on the verge of becoming reality.

IMPROVING PREDICTIONS – Physics Modeling

2. *Physics and numerics of reactive NSE may need to be revisited*

- Physics, assumptions, modeling depend on application context
 - Some common assumptions, e.g.,
 - Local Thermal Equilibrium
 - Perfect gas
 - No radiation
 - Kolmogorov's ("K41") turbulence scaling $(u')^3/\ell = \varepsilon$
 - Eddy diffusivity $\gg$ molecular diffusivity
 -
 - may be standard *or historically motivated*, but are not always true and may affect negatively results
-  when results are unsatisfactory, question and revisit assumption(s), make physical/mathematical models more realistic.

IMPROVING PREDICTIONS – Some smouldering issues

Focus on Numerics and Physics impacting accurate Turbulent Combustion simulation

1. Numerics: Consistency and Convergence

2. Physics (mostly for LES, but also DNS)

2.1 Multi-Component Diffusion (MCD)

2.2 Compressibility

2.3 Turbulence-Chemistry Coupling

2.4 Comparing Predictions and Experiments

3. Conclusions

IMPROVING PREDICTIONS – Consistency & Convergence

1. Convergence of Numerics for Navier Stokes Equations (NSE) hard to prove

- Common assumption: higher order schemes solve NSE more accurately
- In fact: Lax Equivalence Theorem[†] holds, applies to Initial Value, well posed, linear Partial Differential equations

“If a Finite Differences method (FDM) satisfies two of {consistency, convergence, stability} then the third is satisfied”.

- Mathematically, the NSE
 - are cast as I.V. and B.C. problems,
 - are strongly non-linear due to convection, kinetics, coupling, while FDM schemes are *linear*, and
 - solving procedure (sequencing, iterating, splitting...) muddles mathematics of, complicates analysis of convergence
- ➡ No assurance FDM of any order converge to NSE, but, generally, trends are *plausible*; convergence to NSE is replaced by residues

$< \varepsilon$

- ➡ Convergence issue not resolved...

- [†][Lax and Richtmyer, *Comm. Pure Appl. Math.*, 9: 267-293]

IMPROVING PREDICTIONS – Multi-Component Diffusion (1/2)

2.1 “Molecular $\ll$ eddy diffusivity” not generally true, fails for intense turbulence, combustion

- Most CFD simplifies molecular transport, *assumed* $\ll$ turbulent transport
- Experiments at Sandia [Barlow et al, 2012-2013] and elsewhere hint molecular diffusion may affect turbulent transport. Fact: at scales ℓ close to dissipative, transport times have different Reynolds dependence ($Re = l u \rho / \mu$)

	molecular diffusivity	eddy diffusivity
times	$\sim L^2/D_i \sim \ell^2/(D_i Re^{3/2})$	$\sim k/\epsilon \sim \ell^2/(\nu Re)$

suggesting molecular diffusion may be faster than turbulent when Re increases

- Thus physics suggests testing multi-component diffusion (MCD) driven by concentration, temperature and pressure gradients (all of same order)



test impact of MCD in a canonical turbulent combustion problem

Focus: on modeling the diffusion velocity $\mathbf{V}_i$ of each species i

IMPROVING PREDICTIONS – Multi-Component Diffusion

Reactive LES CFD often over-simplifies molecular transport $\mathbf{V}_i$

Species transport equation

$D(\rho Y_i)/Dt = - \text{grad}(\rho \mathbf{V}_i) + \omega_i$

- Accurate Multi-Component Diffusion physics:

$$\mathbf{V}_i = \mathbf{V}_{i,1} + \mathbf{V}_{i,2} + \mathbf{V}_{i,3}$$

- $\mathbf{V}_{i,1}$ = diffusion due to species gradient = $(W_i/\bar{W}) \sum_j D_{ij} \nabla(Y_j \bar{W}/W_j)$
- $\mathbf{V}_{i,2}$ = due to pressure gradient = $W_i \nabla \ln(p) \sum_j D_{ij} Y_j (1/W_j - 1/\bar{W})$
- $\mathbf{V}_{i,3}$ = due to temperature gradient (Soret effect) = $(W_i/\bar{W}) D_i^T \nabla \ln(T)$

- Mixture-Averaged Diffusion model: $\mathbf{V}_i \equiv \mathbf{V}_{i,1} = (W_i/\bar{W}) \sum_j D_{i,m} \nabla(Y_j \bar{W}/W_j)$

- Constant Lewis model: all species have equal thermal, chemical diffusivity

 Test diffusion impact with **DNS** of Turbulent Reacting Mixing Layers

- need to pick a DNS code

Impact of MCD on Turbulent Combustion

Use DNS and a well defined test problem in collaboration with Sandia (J.Chen)

- ▶ Codes and test chosen in collaboration with J. Chen (Sandia), V. Sankaran (UTRC)
- At UTRC: LESLIE (2nd order – run in DNS mode)
- At Sandia: S3D (6th order)
- Test Problem: temporal shear layers
 - if significant, diffusion effects should emerge *regardless of code or scheme order*
- Testing in three steps and using three diffusion models:
 1. Validate: S3D & LESLIE with Mixture-Averaged Diffusion (MAD)
 2. Compare: Mixture-Averaged vs. Multi-Component
 3. Compare: Mixture-Averaged vs. $Le_i = 1$ diffusion model

Impact of MCD on Turbulent Combustion – Test Problem

Test problem: 3D temporal mixing layers

Flow parameters:

- $Re_{\text{Jet}} = 8000$; $Mach = 0.4$
- $Re_{\text{Turb}} = 600$

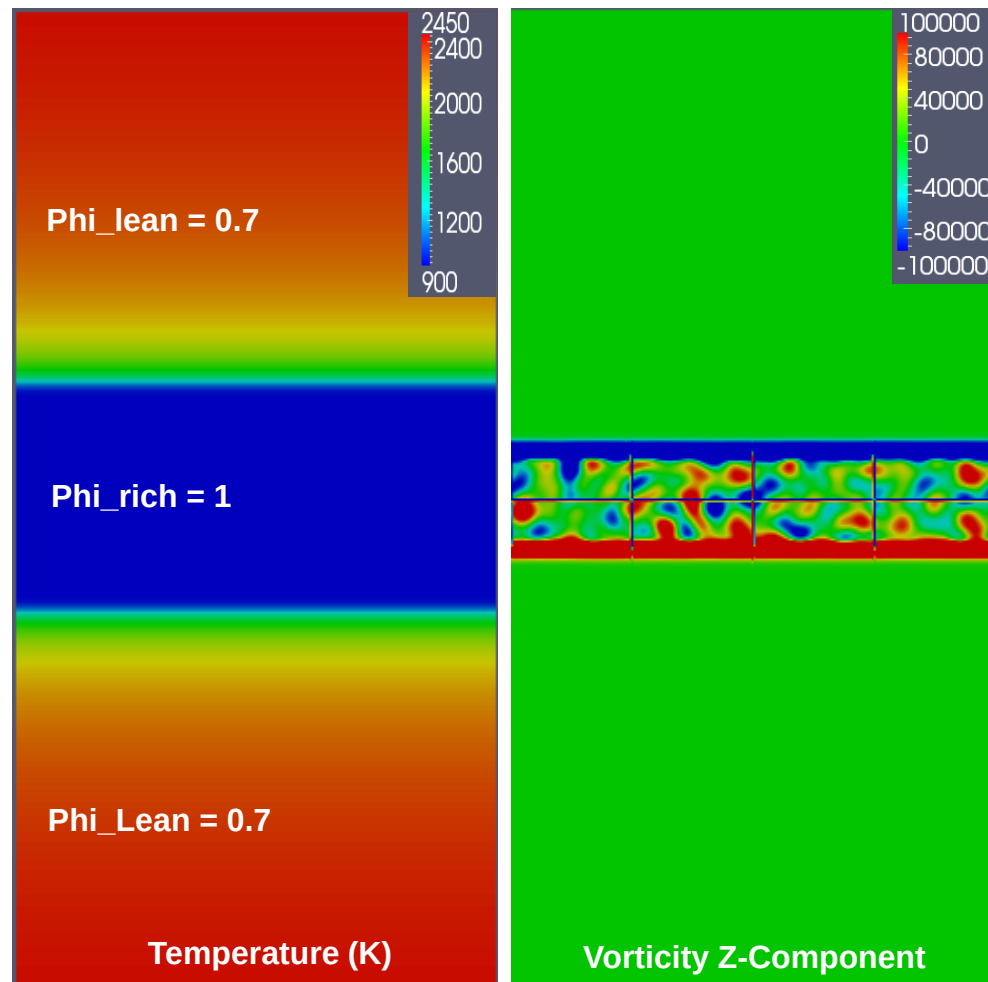
Flame parameters:

- Fuel: $0.5\text{CO} + 0.5\text{H}_2$ syngas
- E.R. = $0.7 \rightarrow 1 \rightarrow 0.7$
- $T = 2430\text{ K to } 900\text{ K}$
- $P = 1\text{ atm}$

DNS Parameters:

- $5H \times 10H \times 3H$; $H = \text{Jet width}$
- $\Delta x = 30\text{ }\mu\text{m}$; $l_k \sim 30\text{ }\mu\text{m}$
- species profile width $\sim 240\text{ }\mu\text{m}$
- $420 \times 600 \times 256$ cells
- Total = 64 Mcells
- Results: averaged over x, z

Initial Conditions

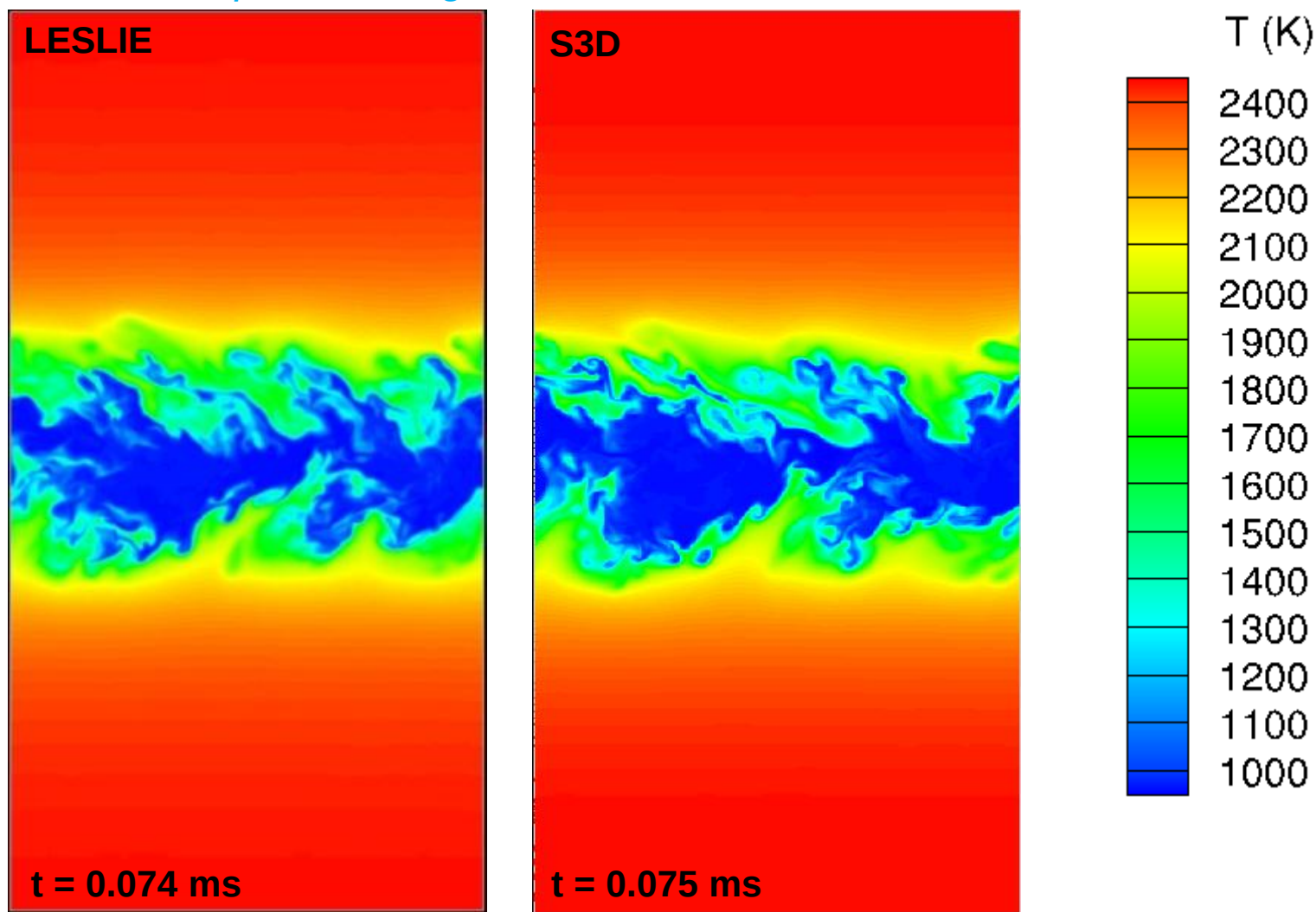


Codes Validation - LESLIE vs. S3D results

Mixture-Averaged Diffusion

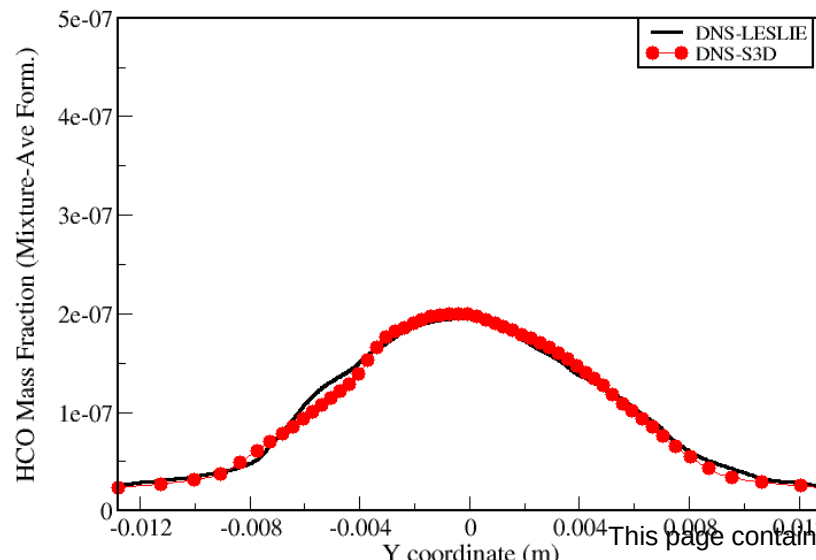
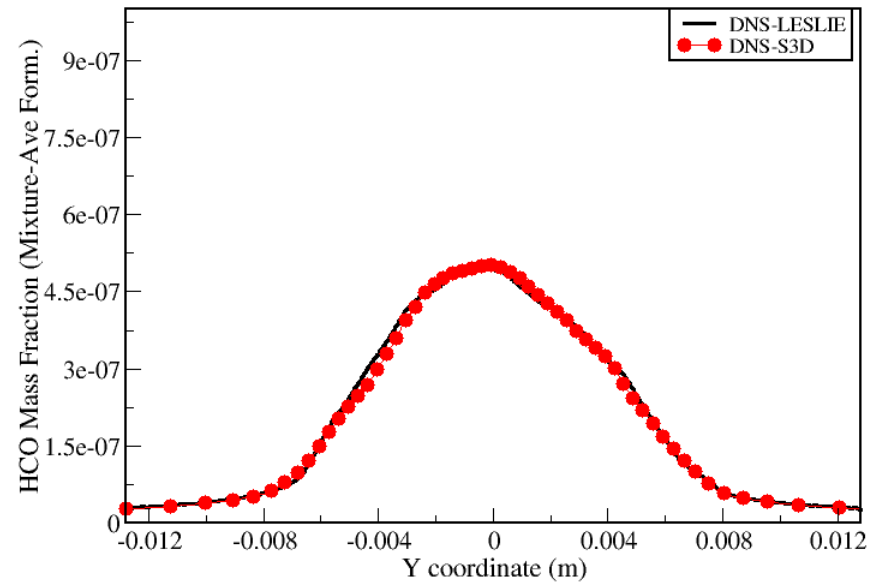
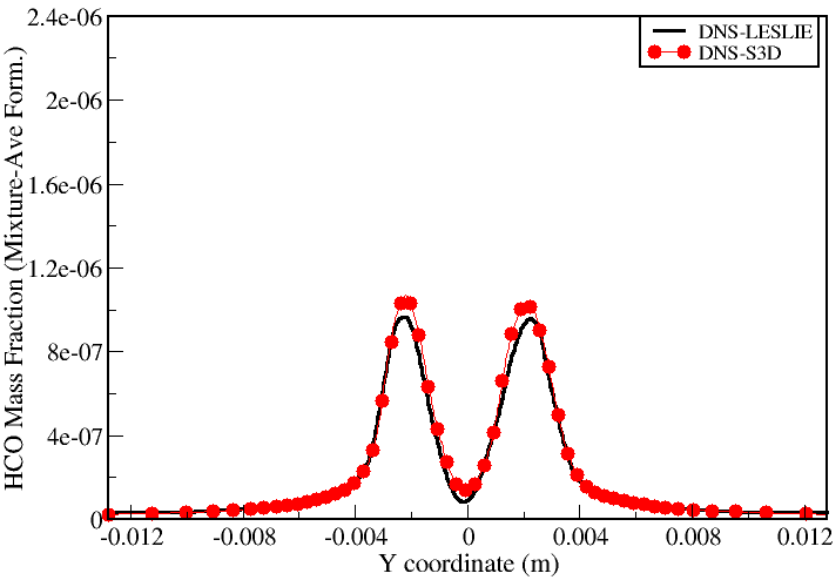
Impact of MCD on Turbulent Combustion

Validation: Reasonable qualitative agreement between S3D and LESLIE



Instantaneous Temperature Field on the x-y plane

S3D (Sandia) vs UTRC LESLIE - HCO at 0.015, 0.075, 0.225 ms

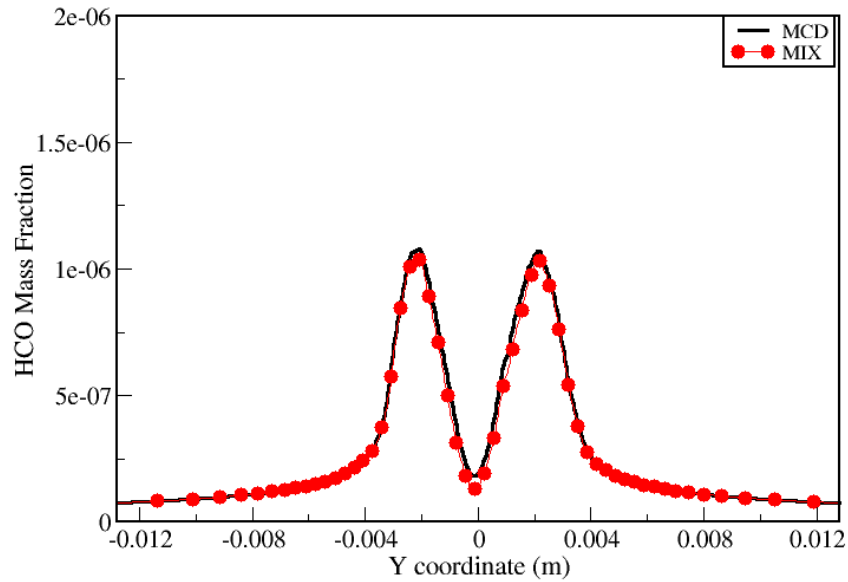


Comparison:

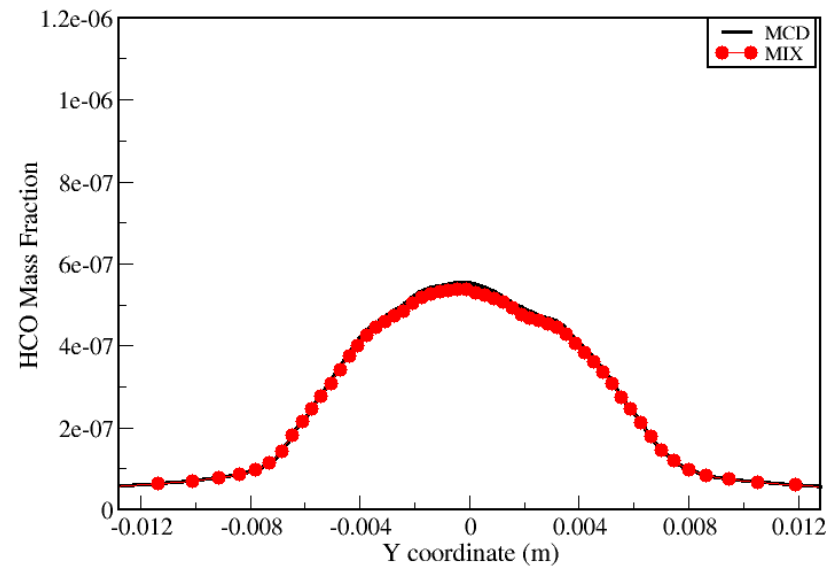
Multi-Component Diffusion
VS.
Mixture-Averaged Diffusion

MCD vs. **MAD**

time = 0.015 ms



time = 0.075 ms



Comparison:

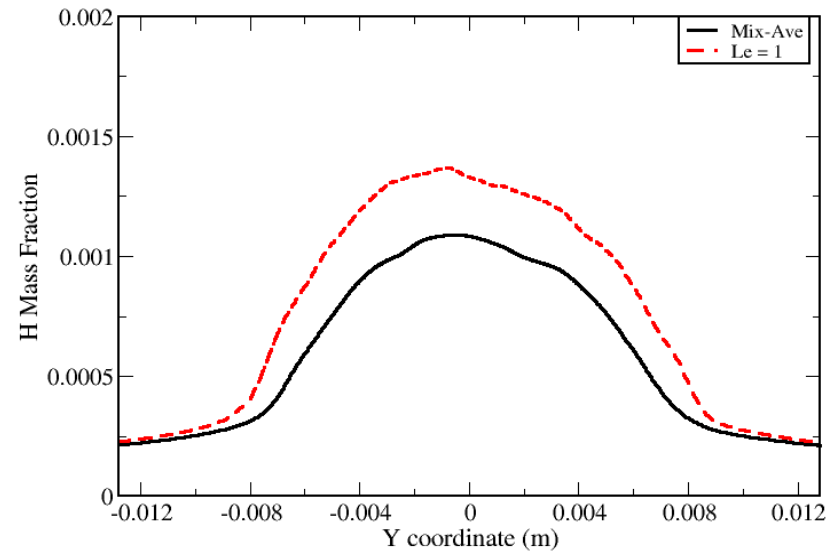
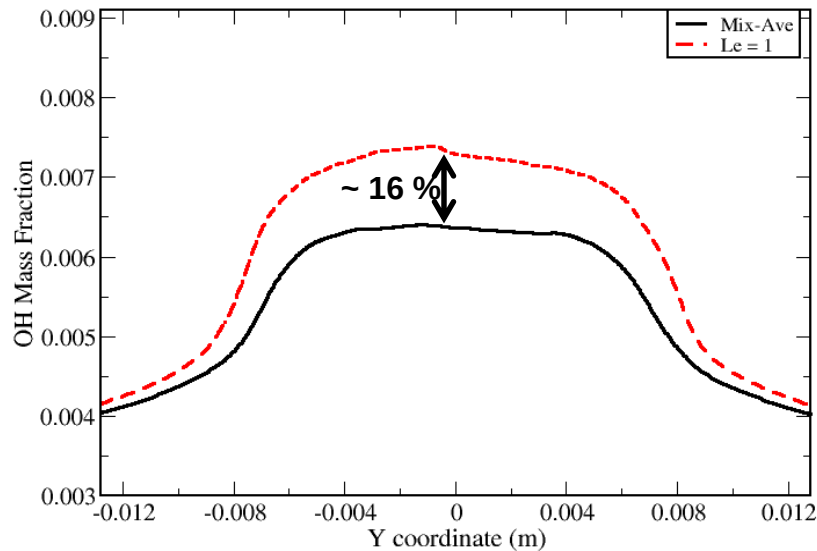
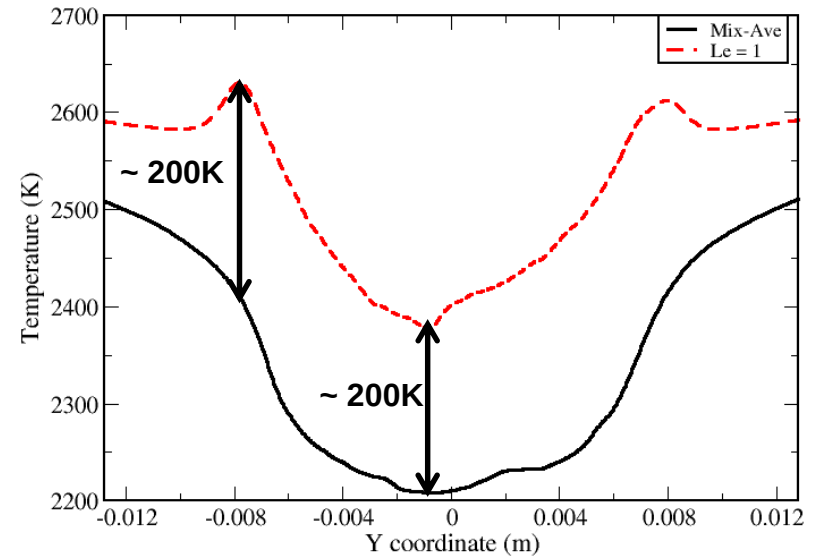
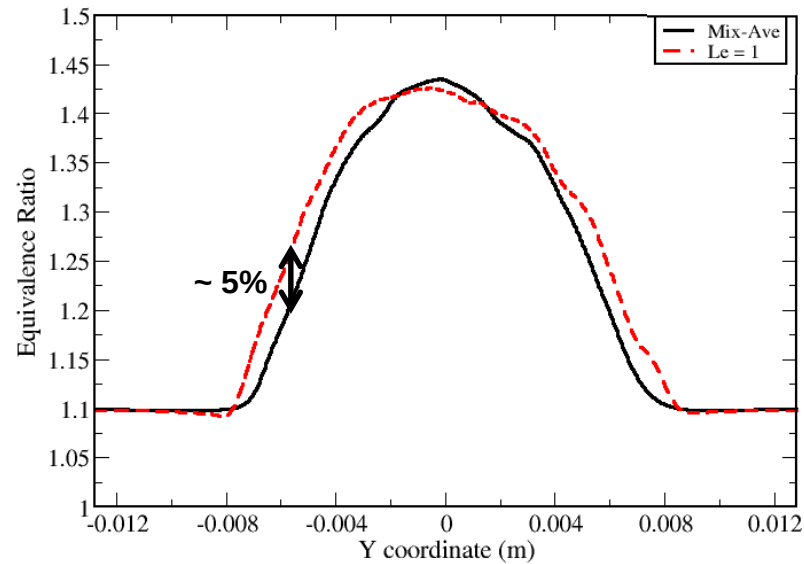
MCD

vs.

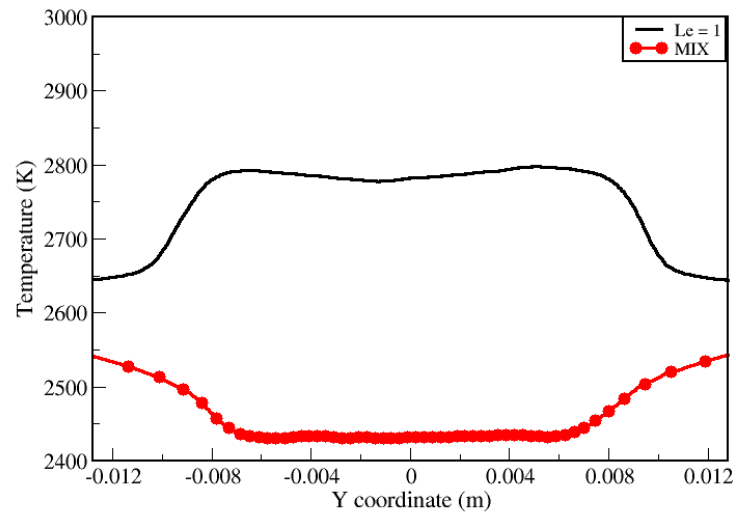
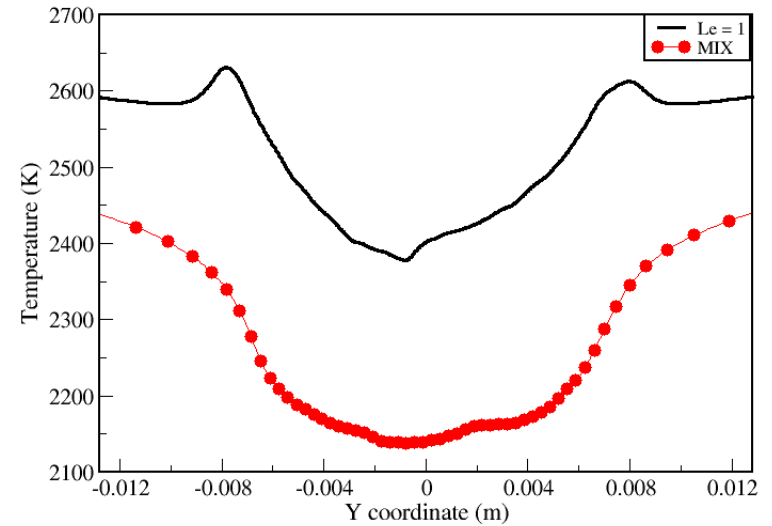
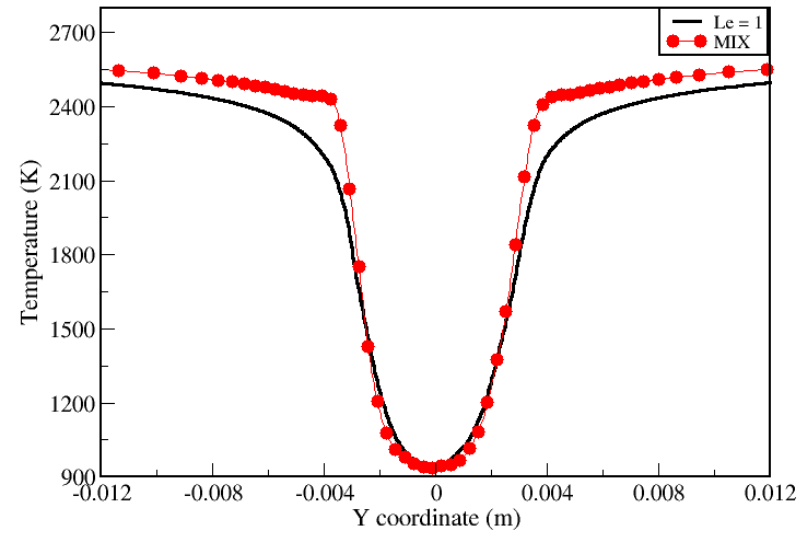
Constant $L_e = 1$ Model

Impact of MCD on Turbulent Combustion

Significant differences between mixture averaged & $Le = 1$ model (e.g., $t = 0.075$ ms)



Full MCD vs. Le=1 Diffusion Model - T at 0.015, 0.075, 0.225 ms



Impact of MCD on Turbulent Combustion

Summary

- ▶ Constant Le used in most CFD codes produces significant Δ compared to the accurate MCD model:
 - $\Delta T \sim 250K$, $\Delta E.R. \sim 5-10\%$; $\Delta Y_i \sim 10\%$ for some endothermic radicals
 - Differences attributable to ΔY_i of radicals with high ΔH_f , (e.g. H, OH) due to 1. kinetics and to 2. **diffusion**
- ▶ Impact of diffusion on turbulent combustion found larger than commonly assumed; must be verified at scale of practical applications

IMPROVING PREDICTIONS – Multi-Component Diffusion (/)

2.1 Other effects of MCD may also be important in some applications

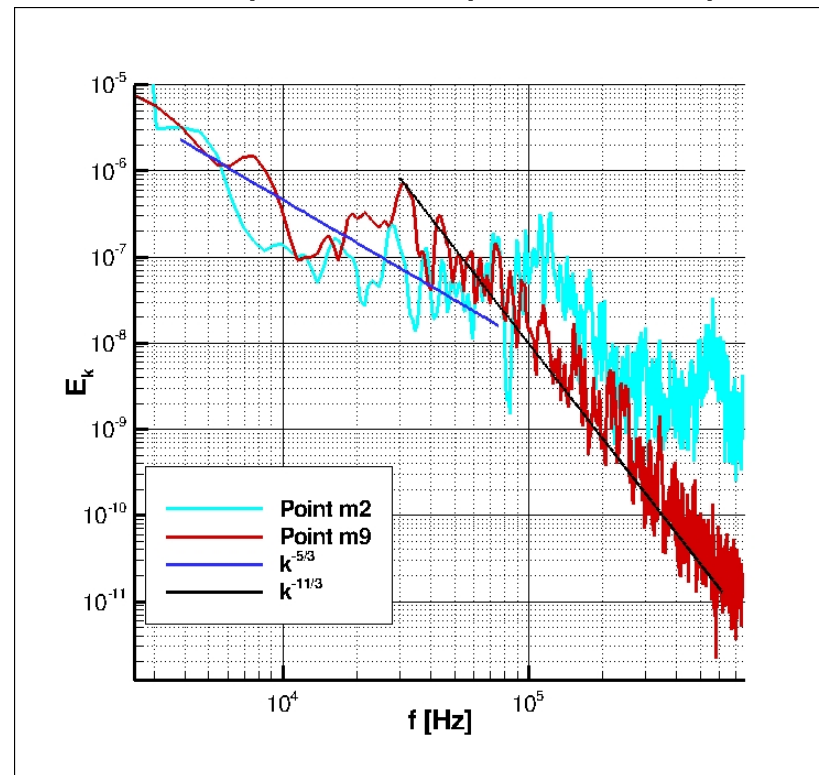
- ▶ MCD includes molecular transport driven by $\text{grad}(p)$
 - $\text{grad}(p)$ effect ~ negligible in incompressible regime
 - $\text{grad}(p)$ effect important in:
 - high Re liquids (cavitation, luminescence)
 - high M flows (enhancing mixing in SCRJ)

- ▶ Molecular transport seems increasingly important with increasing turbulence: see [Tim Lieuwen, Jim Driscoll, AFOSR work 2013-2014]

IMPROVING PREDICTIONS – Compressibility Effects (1/2)

2.2 Kolmogorov scaling fails at $M > 1$, might not always hold also in turbulent combustion

- Motivation: SCRJ modeling (1998-2011) [Ingenito et al, 2010]
- Where compressibility is significant LES results hint at spectral slope $\sim -8/3$ (or $-11/3$) rather than Kolmogorov's $-5/3$
- Physics: K41 derives from ROM analysis of vorticity (ω) equation at low Mach
- The *compressible* ω equation *cannot* yield either K41 or a K41-analog since it contains density: K41 does not, is no longer valid.
- A K41-analog can be derived by including ρ and therefore *thermodynamics*
- Some hints that K41 fails also in flows with large $\text{grad } \rho$ (combustion)
➡ k - ϵ model also not valid...



IMPROVING PREDICTIONS – Compressibility Effects (2/2)

2.2 Kolmogorov K41 scaling failing at $M > 1$ suggested also by dimensional analysis

- Dimensional analysis predicting the E_K spectrum in a $M = 2$ SCRJ flow shows dependence on $k^{-8/3}$, not $k^{-5/3}$ [Ingenito et al, AIAA J., 2010]
- Steeper $-8/3$ slope indicates larger dissipative scales when M^2 is significant
- Proposal to develop compressible analog of K41 invited by AFOSR; to be funded (2015?)
- ▶ Larger dissipative scales may enable DNS of supersonic internal and external flows

IMPROVING PREDICTIONS – Turbulence/Chemistry Coupling

2..3 *Turbulence-Chemistry Interaction may not be fully accounted in LES SGS*

- Research motivated by attempting to improve LES SGS closures (2004-2005)
- Most SGS flame models are ‘one-way’: tell how turbulence affects chemistry
- Physics: Coupling is *two-way*: chemistry does affect turbulence via density. Heat release may increase, or may suppress, turbulence
- Evidence: poor LES predictions of turbulent reacting flows.
Due to solvers, closures, most SGS models may only partially account for conversion of heat release to turbulent KE and vorticity:
coupling may be mostly “one-way”
- ▶ Is there a way to ‘tighten’ the heat release-turbulence coupling?
2004-2005 work suggests a way based on Crocco-Vaszony equation

IMPROVING PREDICTIONS – Turbulence/Chemistry Coupling

2..3 Turbulence-Chemistry coupling in LES enforced using Crocco-Vaszony equation

■ The Crocco-Vaszony (C-V) equation

$$\frac{\partial \mathbf{V}}{\partial t} - \mathbf{V} \times \boldsymbol{\omega} = T \nabla s - \nabla h_t - \frac{1}{\rho} \{ (2/3) \nabla (\mu \nabla \cdot \mathbf{V}) + (\nabla \mu) \cdot [\nabla \mathbf{V} + (\nabla \mathbf{V})^t] + (\nabla \mu) \cdot [\nabla \mathbf{V} + (\nabla \mathbf{V})^t] + \mu [\nabla^2 \mathbf{V} + \nabla (\nabla \cdot \mathbf{V})] \}$$

tells that changes of velocity and vorticity are linked to heat release.

- C-V can generate SGS closures. For instance *analytical work* shows the filtered energy equation has an explicit SGS *source of kinetic energy*

$$\mathbf{S} \equiv \partial(\mathbf{V}^2/2)/\partial t = F(s, q, \nabla h_t, \mathbf{V}_i, \Phi, \mu, \rho)$$

- C-V closure tested successfully in 3-D axisymmetric flow [Parisi et al, 2005] using the Sidney jet burner experiment [Masri et al, 2002]:

3D Reactive Case: Source Distribution (5/10)

- Source term **S**:

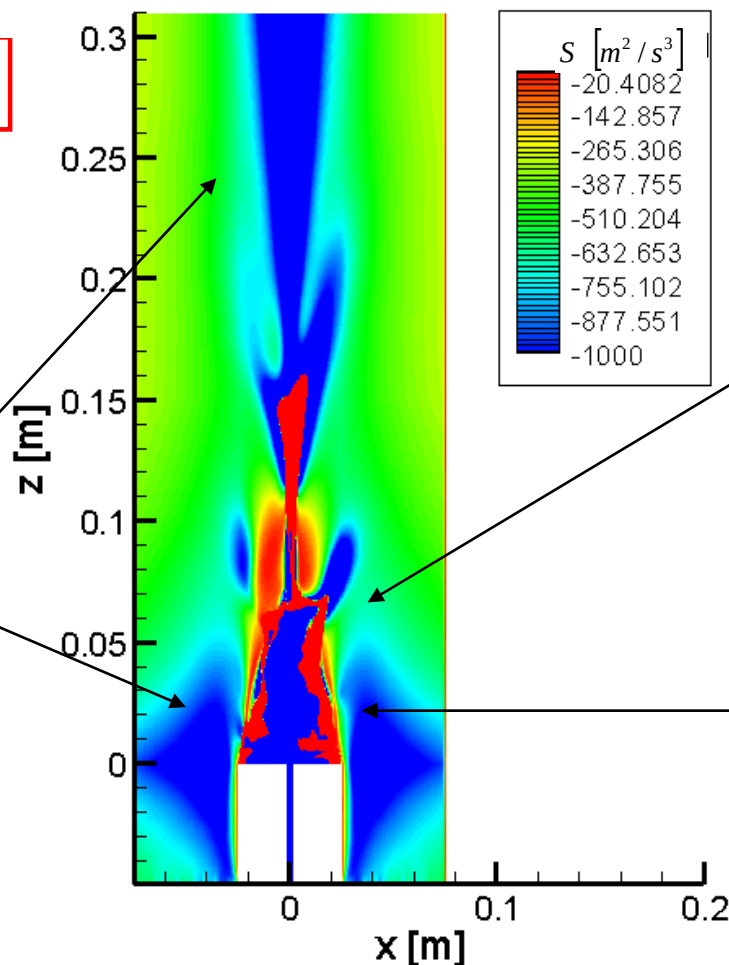
⇒ may be **positive** and **negative** ⇒ combustion can produce kinetic energy (backscatter). S field different than in the “cold” case: **S** depends on combustion

$$S [m^2 / s^3]$$

Non reactive zone:

Viscous
Dissipation of
kinetic energy

(Field snapshot)



Reactive zone:

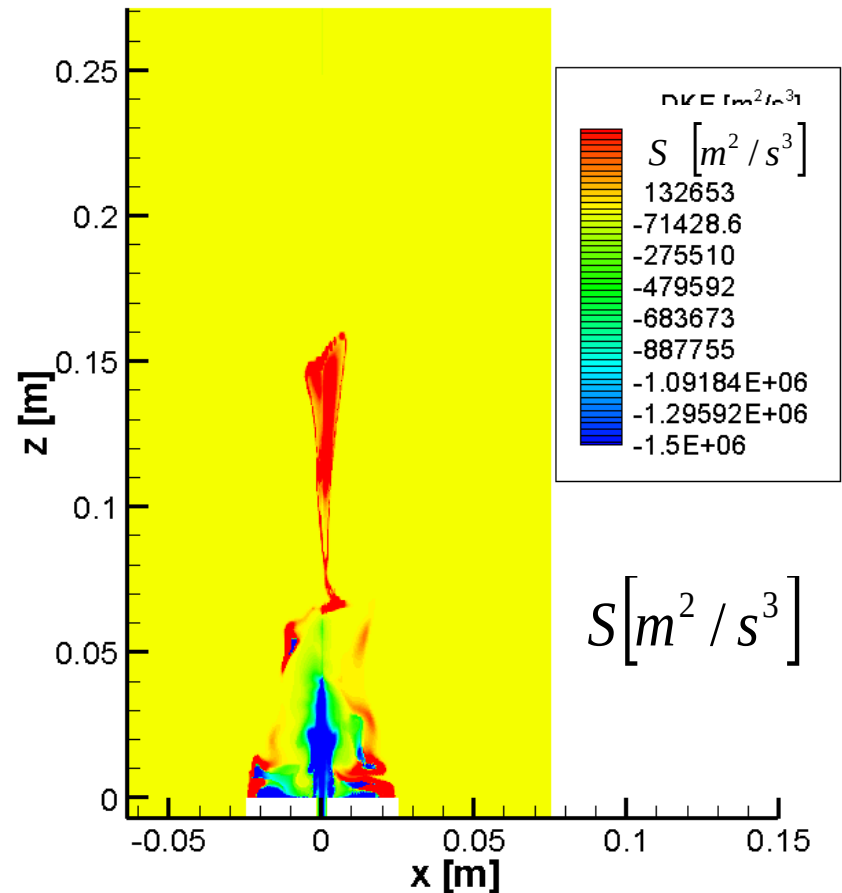
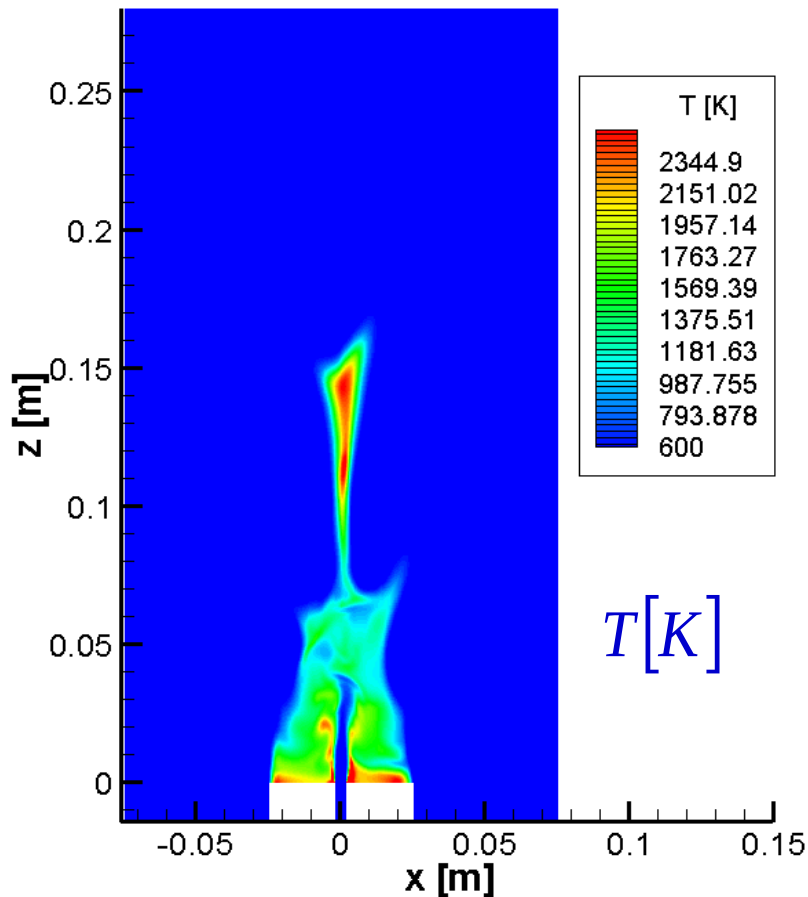
Production of
kinetic energy by
combustion

Viscous
Dissipation of
kinetic energy

Comparison Between Temperature and S Fields (6/10)

- **S** depends mostly on **chemical reactions** $\Rightarrow$ depends on **T**
 $\Rightarrow$ **S** and **T** have similar fields!

(Field snapshot 1)



IMPROVING PREDICTIONS – Turbulence/Chemistry Coupling

2.3 SGS closure using Crocco-Vaszony approach has pluses and minuses

■ ADVANTAGES:

- Can account for subtler effects (e.g., due to diffusion).
- Can generate SGS closures consistent with NSE
- Includes entropy explicitly, so the Second Principle can be implemented
- Avoids the recourse to ‘eddy viscosity’ to close equations

■ DISADVANTAGES:

- Higher mathematical complexity and computational cost
- Uses not too familiar gas dynamics
- Absence of μ_T may drive numerical instability

IMPROVING PREDICTIONS - Predictions vs. Measurements

2..3 Comparisons must account for type of variables and type of diagnostics

- FANS and density-filtered LES produce *mass-averaged* variables
- As is, *most* optical diagnostics (CARS, Raleigh...) produces *time-averaged* data



comparisons *may* be inconsistent , for instance

mass averaged V consistent with LDV, hot wire measurements

mass averaged T not consistent with CARS measurements

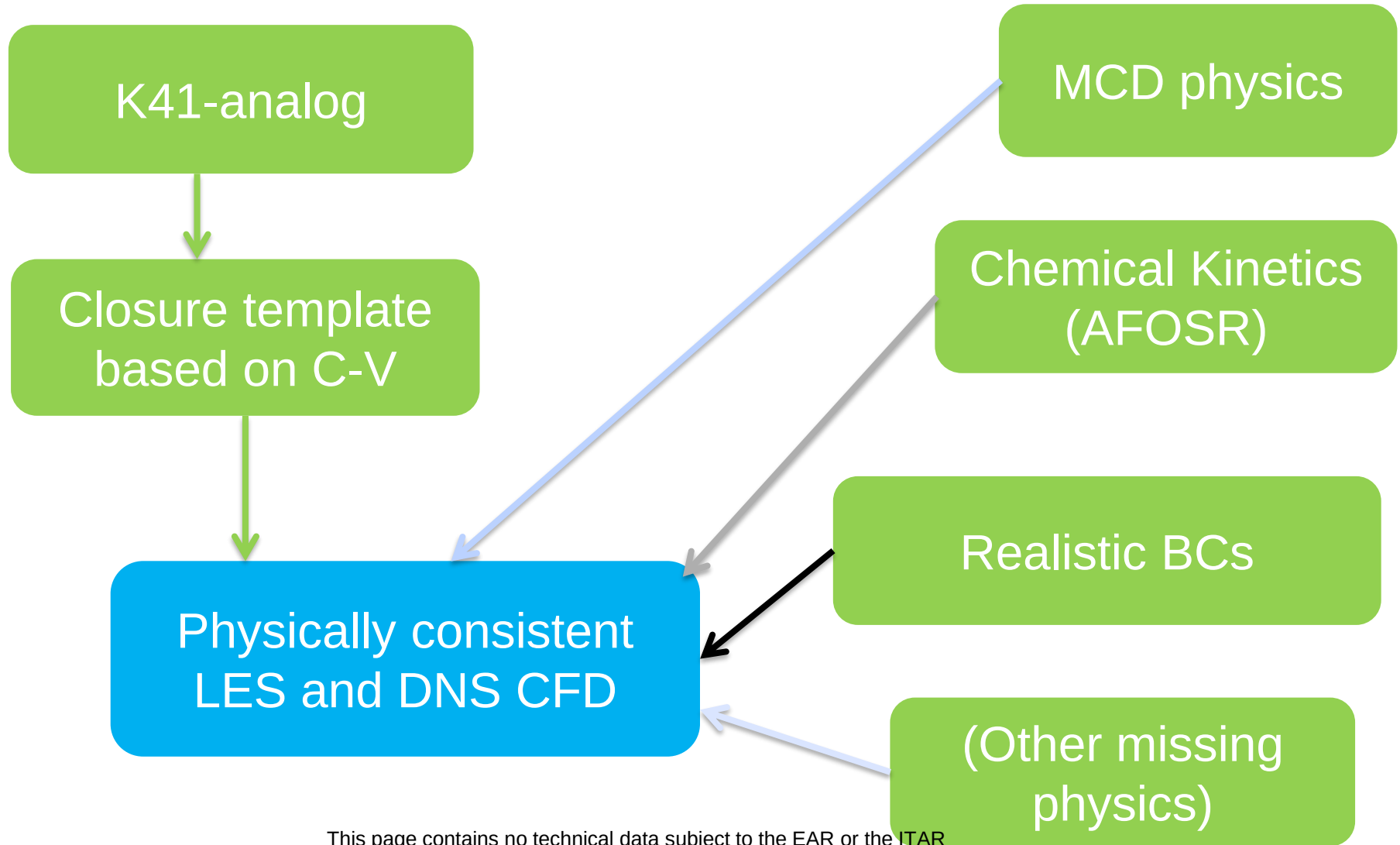
- ▶ Data may have to be post-processed for a fair comparison

[P A Libby; H A Becker in: "Studies in Convection", ed. by B E Launder, Academic Press, p.4; p. 45 et seq., 1977] ; Greenhalgh (1987); N. Venkat (1990s)

- ▶ *A numerical modeler should know the measurements he/she is using better than who took them*

CONCLUSIONS (1/2)

A personal blueprint of a LES fidelity-improving plan (round 1...)



CONCLUSIONS (2/2)

3. *Turbulent combustion simulation fidelity needs revisiting models, assumptions*

- Resources should be invested in the numerical convergence issue
- *Other issues* exist affecting fidelity, e.g.,
 - Local Thermal Equilibrium validity
 - radiation impact on turbulence
 - kinetics at Mach > 1 (for SCRJ)
 - ...
- This talk is meant not only to stimulate interest in them, but also...
- ...more generally, to question assumptions and routine ways of doing things

Back-up

GOALS

Research goals may differ depending on context

Different organizations understand “improving” differently:

	INDUSTRY	SCIENTIFIC ORG
Need to predict...	Trends	Numbers
Timing:	O(1) month	O(1) year
Operating Cost:	High	Medium/Low



Here emphasis is on impact of numerics and physics on simulation fidelity