Mapping turbulent combustion

by Brian Spalding

Melbourne
2011

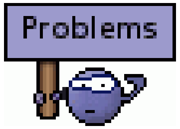
Ninth Australian Heat and Mass
Transfer Conference 2011

Part 1: 25 centuries of CFD & HMT in 25 minutes: from conventional to populational

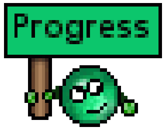
Each slide will have four parts:

what was the basic idea

what benefit it was expected to confer



why things did not work out quite as had been hoped



how nevertheless something good transpired

Archimedes (267 BC)

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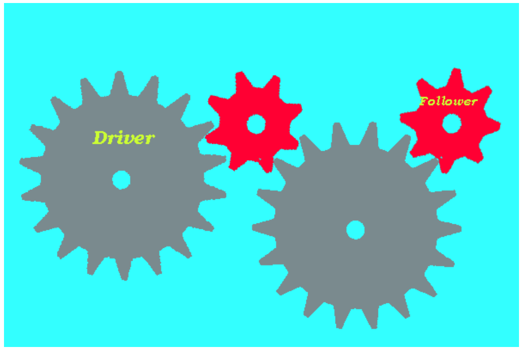
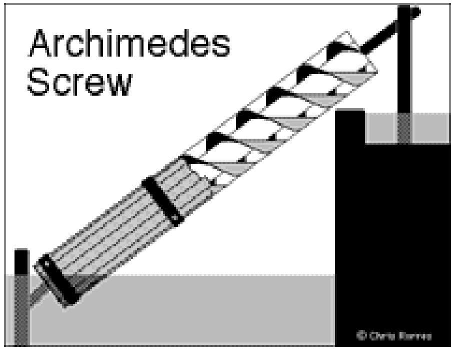
Proposal Give me a lever and a rock to rest it on,

Promise THEN I will move the world.

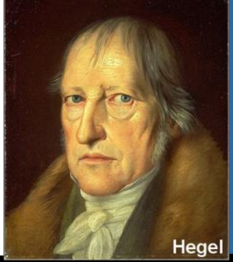
Problems No suitable rock.

Progress BUT... we have the wheel-barrow, and gear trains and the Archimedean spiral pump which causes **swirling flow**.





Newtonian extrapolators: determinist philosophers



Proposal

Tell us the **initial position** and **velocity** of all molecules,

Promise

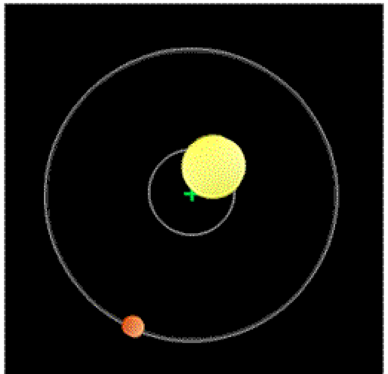
THEN Newton’s laws will **determine everything** that follows.

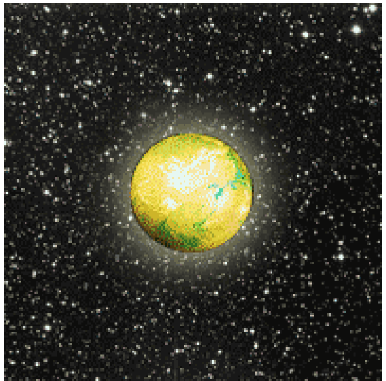
Problems

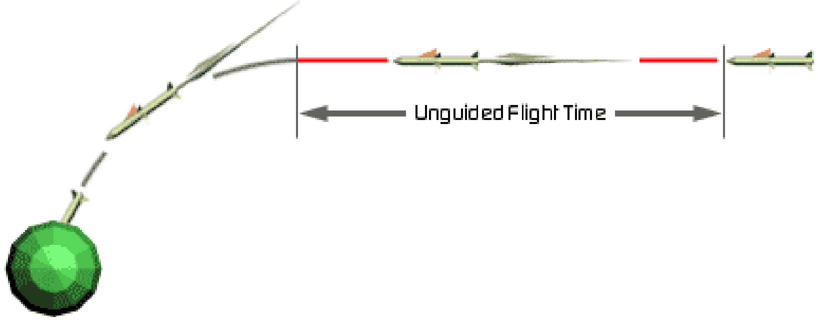
Too many molecules!

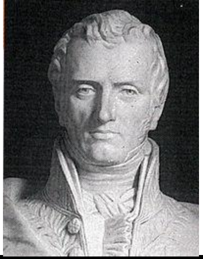
Progress

BUT... we **can** predict movements of planets and moons; and of ballistic missiles.

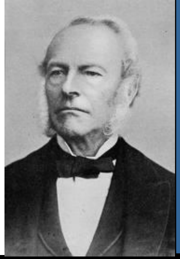








Navier and Stokes



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Proposal

Suppose we can treat fluids as **continua**, fully characterised by **density** and **viscosity**,

Promise

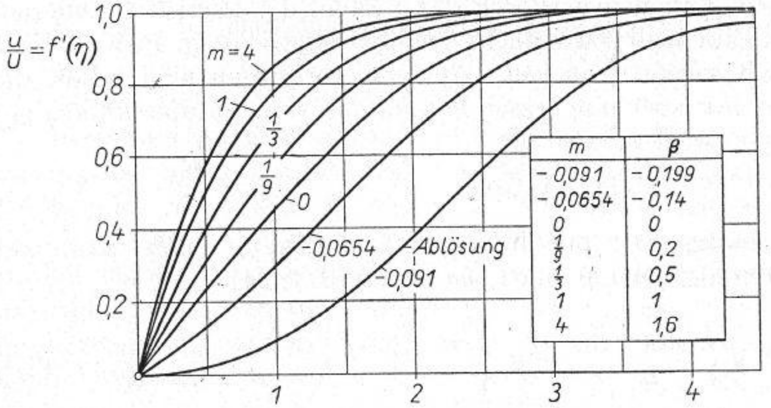
THEN solving **our** equations will predict **all fluid flows**.

Problems

Analytical solution methods were **not powerful** enough, **numerical** methods too **costly**.

Progress

BUT... **simple flows** could be analysed, *e.g.* laminar **boundary layers,** wakes and jets.

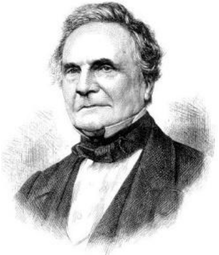


m	β
−0,091	−0,199
−0,0654	−0,14
0	0
$\frac{1}{9}$	0,2
$\frac{1}{3}$	0,5
1	1
4	1,6

Velocity profiles in laminar boundary layers on wedges of various angles

$$\eta = \sqrt{\frac{m+1}{2}}\sqrt{\frac{U}{\nu x}}\,y$$

Charles Babbage



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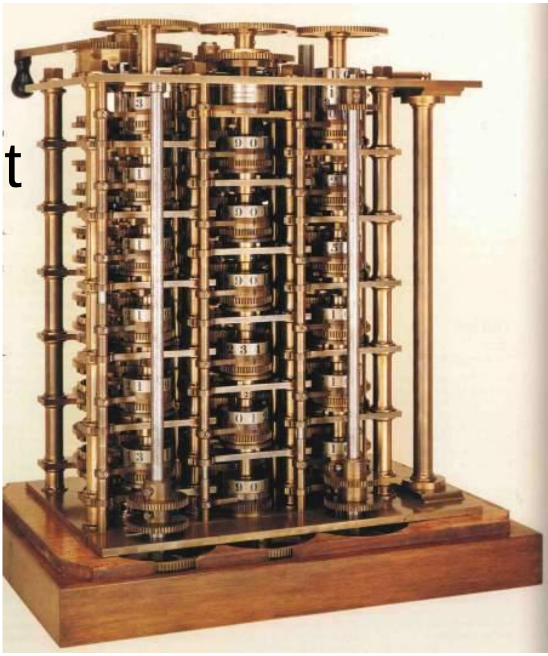
Proposal

I can **build a machine** consisting of (Archimedean!) gear-wheels and levers;

Promise

THEN it will do **numerical** calculations **mechanically,** *i.e.* without human labour.



Problems

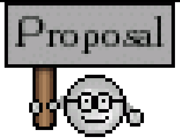
It would have needed 25,000 parts, weighed 13,600 kg, been 2.5 m tall.

So it was started, but **never completed.**

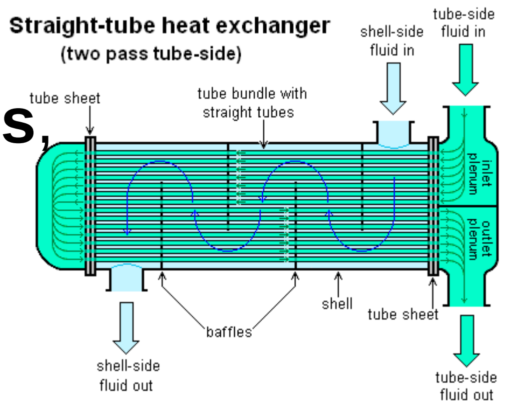
Progress

BUT it paved the thought-way for the **electronic digital computer.**

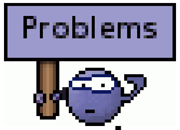
Heat-exchanger and furnace designers



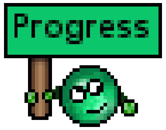
Give us values of heat-transfer and friction **coefficients**,



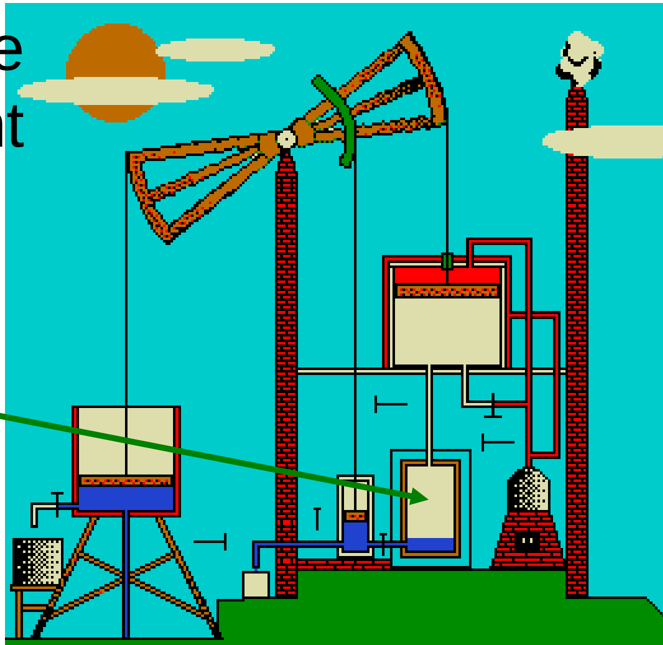
THEN we will tell you how much **surface** your equipment needs and how much **pumping power**.



The coefficients could be known only **after** the equipment had been built.



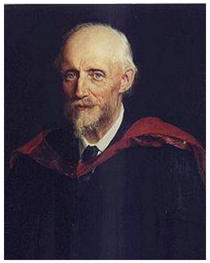
BUT.... James Watt built his separate condenser in 1765 **without** such knowledge; And so greatly accelerated the Industrial Revolution.



Experimentalists using Similarity Theory

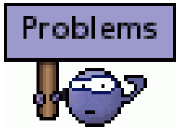
Similarity theory predicts **full-scale** performance from **laboratory-scale** measurements.

SO design engineers can use our data when expressed in terms of **Reynolds, Nusselt** and **Prandtl** numbers.


Reynolds

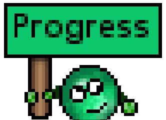

Nusselt


Prandtl



Experiments are **expensive**; and never numerous enough.

Moreover similarity requirements sometimes **conflict**.



BUT correlation-based predictions **are better than guesses;** so they are used by engineers (with caution).

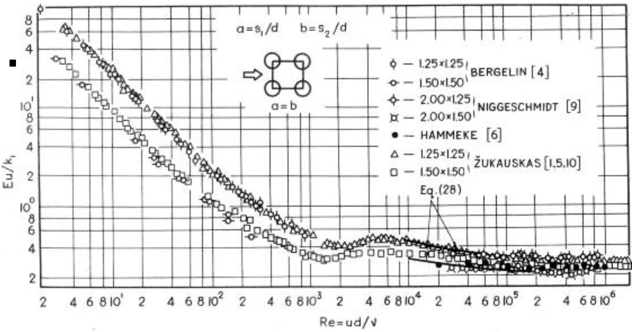


Figure 7 Pressure drop of in-line banks.

For $(b-0.8)/(a-1) \leqslant 1$:

$$\mathrm{Eu} = 0.52\left(\frac{b-0.8}{a-1}\right)\mathrm{Re}^{r} \quad (29)$$

The exponent r is given by

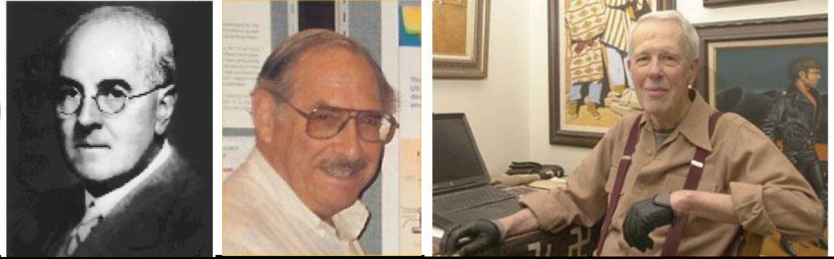
$$r = 0.12\left(\frac{b-1}{a-1}\right)^{0.5} \quad (30)$$

2. Equations for staggered, equilateral triang
banks

For $6 \times 10^2 < \mathrm{Re} < 7 \times 10^3$:

$$\mathrm{Eu} = 1.42\left(\frac{1}{a-1}\right)^{0.33}\mathrm{Re}^{-0.15}$$

For $7 \times 10^3 < \mathrm{Re} < 2 \times 10^5$:



CFD pioneers

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Proposal

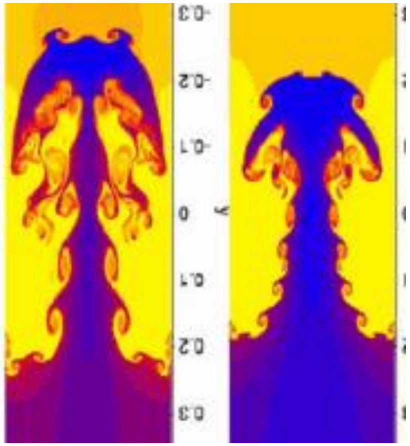
We have **digital computers** and **Navier-Stokes** equations;

Promise

SO we will **compute** the coefficients and the flow patterns; and **experiments** will be **less needed**.

Problems

Small-scale, **rapidly** fluctuating eddies (**turbulence**) govern friction and heat transfer; so the grids required are **impossibly fine**.



Progress

BUT... at least **laminar flows** could now be computed more reliably, **swiftly** and **cheaply** than they could be investigated physically.

Turbulence modellers: Boussinesq, Prandtl, Kolmogorov

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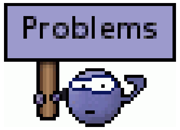
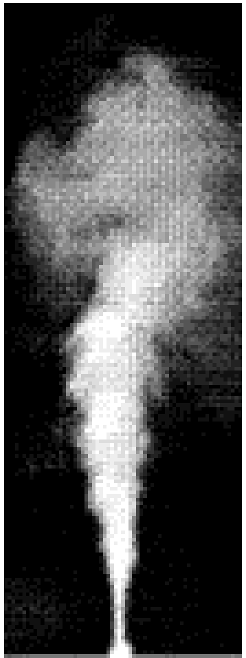
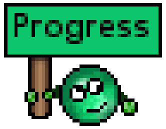
Suppose turbulent flows differ from **laminar only** *via* **enlargement** of **effective viscosity**,

THEN **our** equations will **calculate** effective viscosity ; so **turbulent** flow **can be predicted** too.

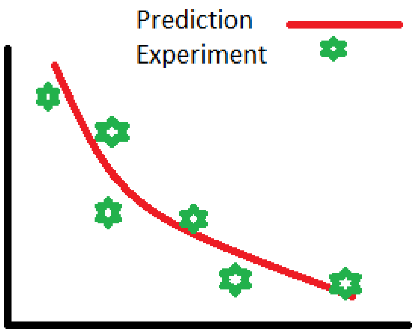


Turbulence **entails more** than enlarged viscosity; and **no model** yet predicts correctly the ‘spread angle’ of **both** plane and round jets.





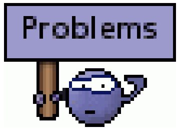
BUT... predictions are often **good enough**, especially when **'calibrated'** using experimental data.



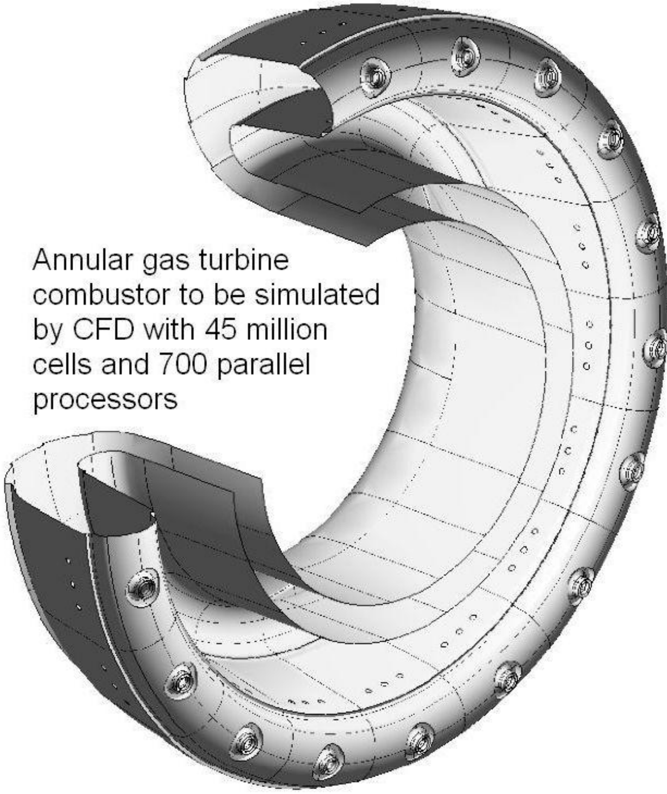
Manufacturers of compressors, turbines, combustion chambers

We will employ those ‘good-enough’ methods in (don’t-count-expense) computations; and

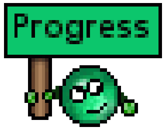
THEN design and build **efficient, cheap, reliable** combustors, turbines, *etc.*



Conventional CFD is **never** 100% reliable, especially for **swirling** and **chemically-reacting** flows;



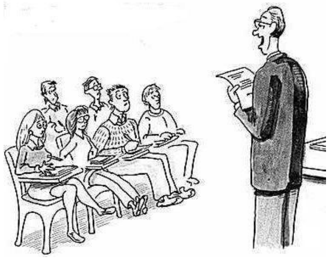
Annular gas turbine combustor to be simulated by CFD with 45 million cells and 700 parallel processors



BUT... it provides at least **some** guidance; so CFD software is widely used by engineers.

MOTS modellers
(MOTS = More Of The Same)

Proposal If we add **more complication** to our models, *e.g.* **Reynolds** stresses, **Large-Eddy** Simulation



Promise THEN surely we shall make **better** predictions (or so our **professors** tell us).

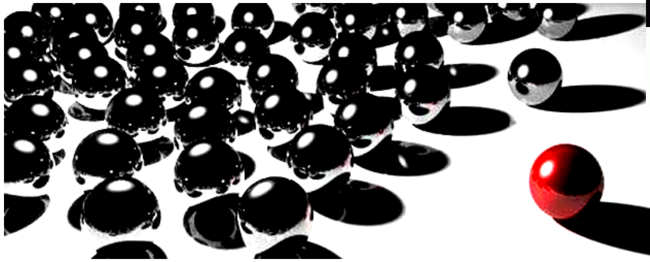
Problems Computational expense increases greatly, but **realism scarcely at all.** Why? **'More-of-the-same'** still **omits** the essential **population-like** character of turbulence.

Progress BUT **close observers** of turbulent flames could see clearly that a single location is occupied by a **population** of **very different** gases at different times.

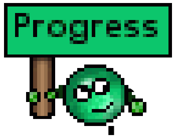
‘Populational-CFD’ innovators

Treating turbulence as a **population-at-each-point** phenomenon must enhance realism,

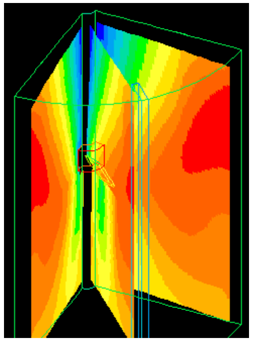
SO **discretising population space** as well as distance and time will allow different reaction rates of population elements, to be distinguished.



!Innovators are far fewer than **‘more-of-the-same’**-ers.

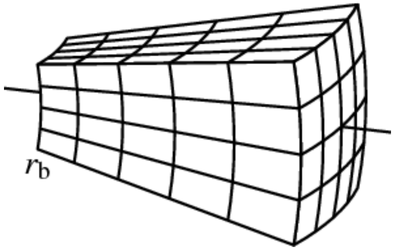


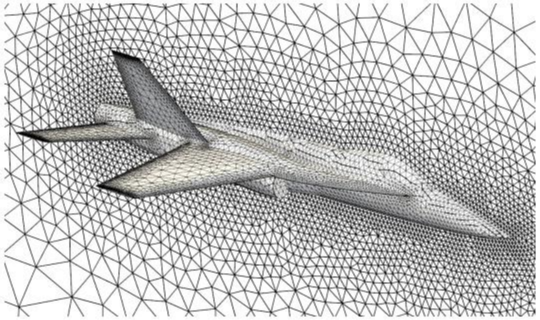
BUT practicability and plausibility of new ideas **have** been demonstrated, *e.g.* for chemical-industry reactors.



How Populational CFD differs from Conventional CFD: 1/9

Both discretise space and time by use of grids of cells, **structured** or **un**structured.





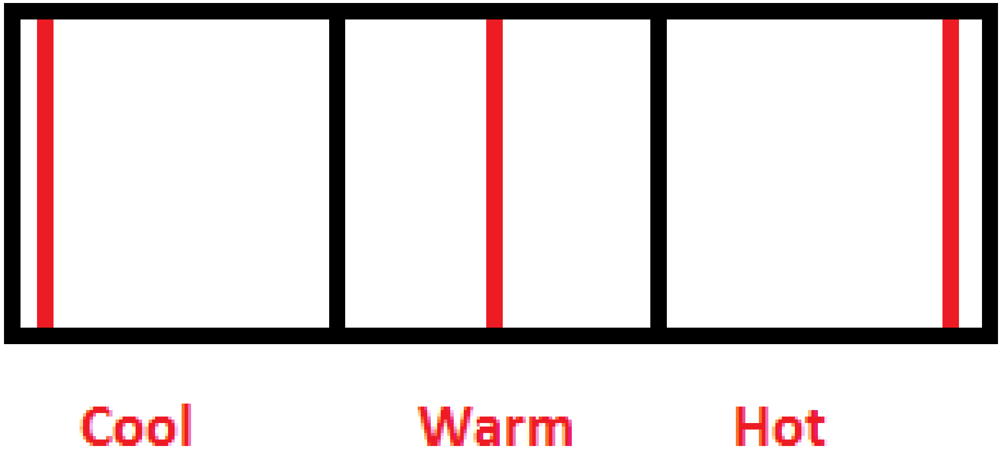
Both solve algebraic mass-, momentum - & energy-**conservation** equations by iterative numerical methods

$$e_P = a_P \phi_P - \sum_{i=W,E,S,N,L,H} a_i \phi_i + a_T \phi_T + b$$

Both take account of **(1) sources, (2) diffusion, (3) convection** and **(4) time-dependence.**

How Populational CFD differs from Conventional CFD: 2/9

Here conventional CFD represents 3 neighbouring cells in a structured grid, with 1 temperature for each cell.

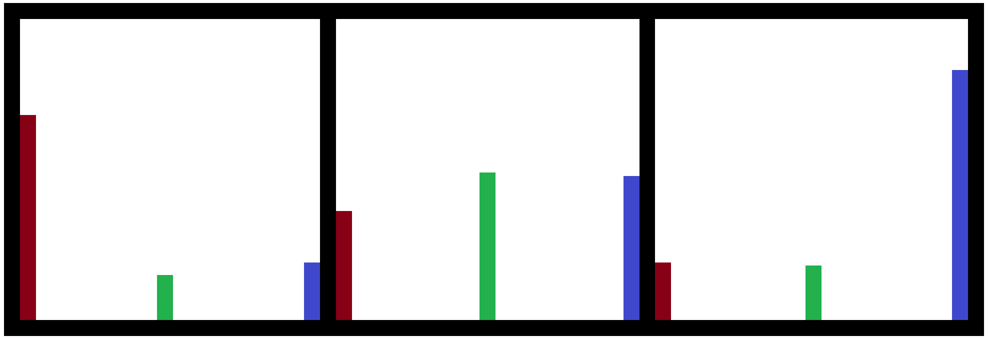


Horizontal position of vertical red lines indicates temperature; with low on the left and high on the right.

Populational CFD (next slide) shows the same by **discretising temperature**, stating **how much** fluid of **each** temperature is present.

How Populational CFD differs from Conventional CFD: 3/9

Here **populational** CFD represents 3 neighbouring cells in a structured grid with **three** temperatures for each cell



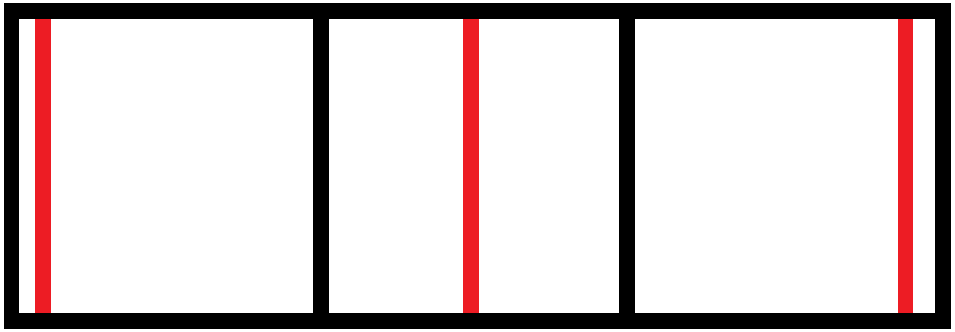
Each cell has **some** cool, warm and hot fluid in it, but **proportions** differ. These proportions are measured by the lengths of the brown, green and blue lines.

The cell-average temperature is equal to the **weighted mean** of the three discrete temperatures of the fluid population.

PopCFD contains all information of ConCFD and **more:** ***viz.* distributions.**

How Populational CFD differs from Conventional CFD: 4/9

Let **time** be the independent variable increasing from left to right: as does temperature, So **a heat source** exists.



Chemical-reaction heat sources vary strongly with temperature. So different members of the turbulent **population react at different rates.**

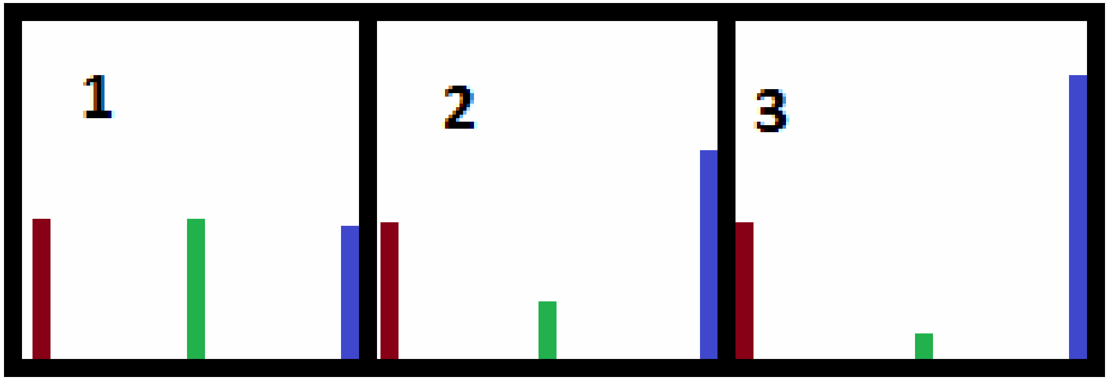
Conventional CFD cannot reflect this.

Populational CFD has come into existence for the reason that:.

Conventional CFD **cannot simulate turbulent combustion**.

How Populational CFD differs from Conventional CFD: 5/9

Populational CFD can recognise that: brown fluid is **too cold** to burn and blue is **already** burned; but green **can** burn.



So **brown** height stays constant with time, **green**’s diminishes and **blue**'s grows by the same amount.

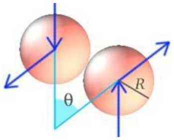
To use three temperatures is insufficient; but even **as few as three** is better than **conventional** CFD’s **one.**

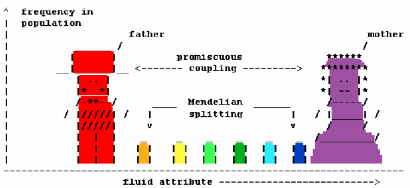
Populational CFD **can simulate turbulent combustion.**

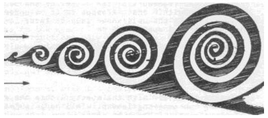
How Populational CFD differs from Conventional CFD: 6/9

Conventional CFD accounts for **four** processes, (sources, diffusion, convection & time-dependence); but Populational CFD accounts for **two more**:

(5) **Merging**, by way of **collision**, **coupling-and-splitting** or **engulfment**, which influence **turbulent combustion**, and







(6) **differential (*i.e. selective)* convection**, **which** influences **buoyant** and **swirling flows.**

The next slide explains item (6).

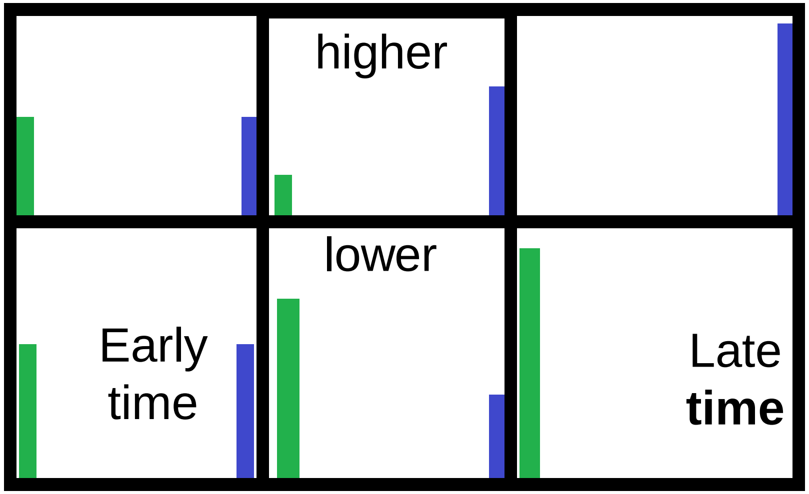
How Populational CFD differs from Conventional CFD: 7/9

Even a **two**-member population can explain the well-documented (but woefully ignored) **body-force-induced un-mixing** process.

This is encountered in **buoyant** and **swirling** flows.

As time proceeds **green** fluid moves down and **blue** fluid up.

Differential convection in vertical direction. 2 members (green & blue) with differing body forces: buoyancy; or centrifugal force in swirling flow.



The discretized variable could be:

- temperature in buoyancy-driven flow

or

- circumferential velocity in swirling flow.

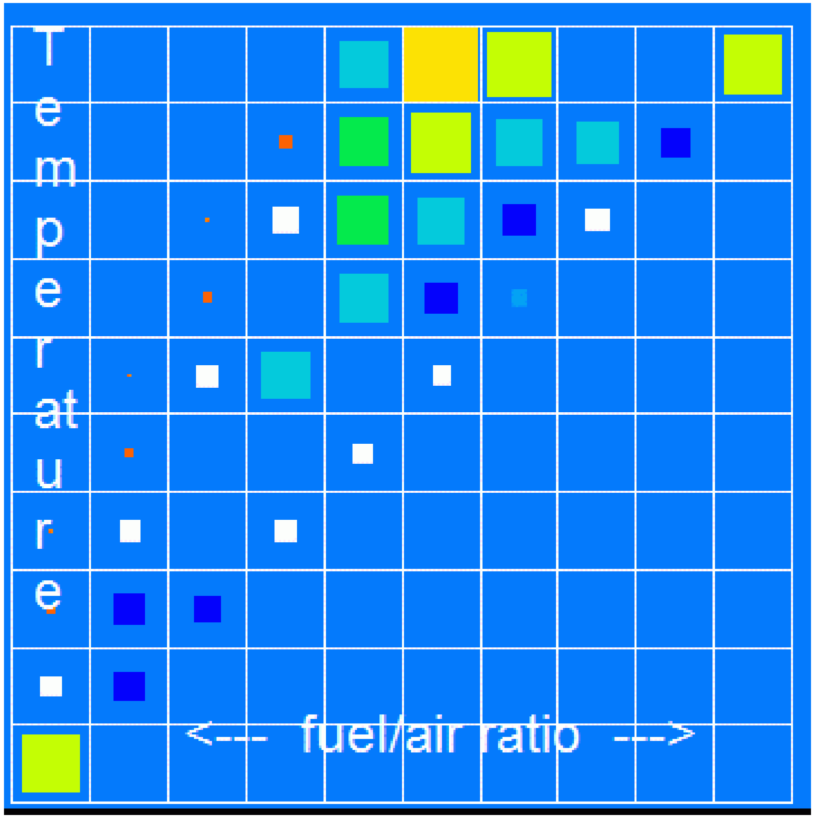
How Populational CFD differs from Conventional CFD: 8/9

Those populations (of temperature and circumferential velocity) were **one-dimensional**. But one may choose to discretise **two** (or more) variables.

Example1. For combustion**:**

10 temperature and 10 fuel/air ratio intervals in **each** x~y~z~t cell.

The **sizes** of squares in each population-grid cell show the **proportions of time** the fluid is in each state.



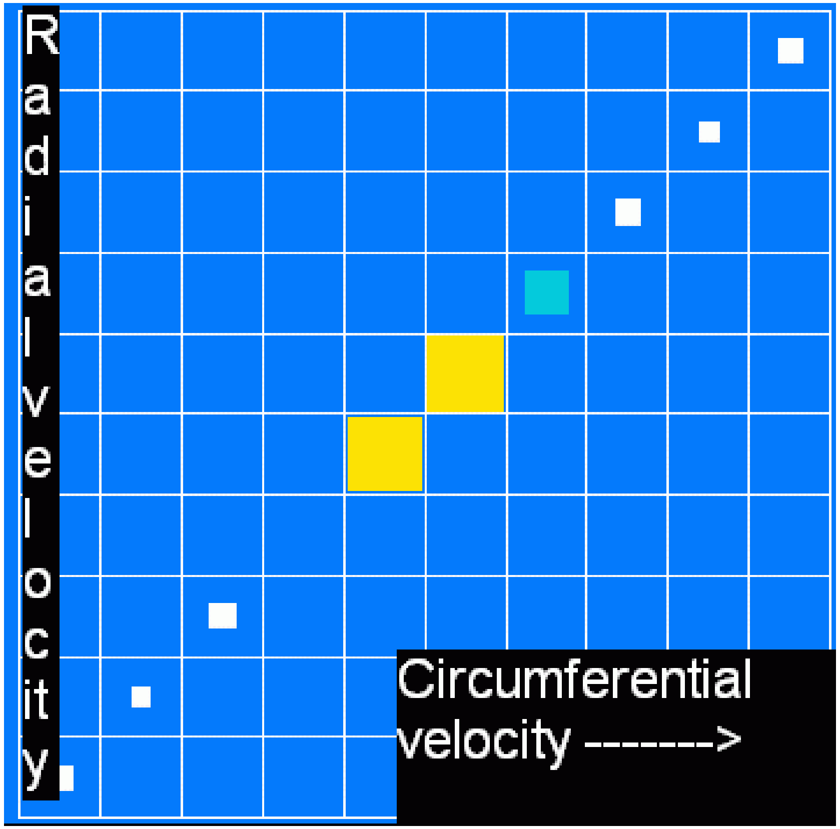
How Populational CFD differs from Conventional CFD: 9/9

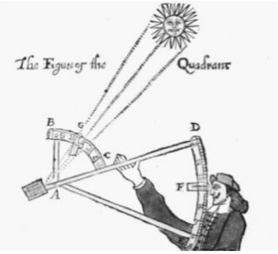
Example 2. For swirling flow, one might choose to discretise the **circumferential** and **radial velocity** components.

The population distribution **might** look like this. Centrifugal force causes **high radial** velocities.

But this is a **guess**; for no-one has yet done the calculations!

Who will be **the first** to do so?





Turbulence cartographers

Proposal

"Give me the map there", commanded King Lear (act 1, scene 1);

Promise

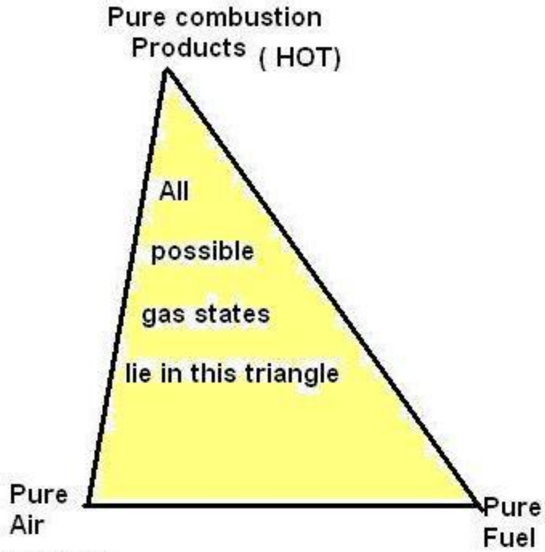
THEN hoped to distribute the **three parts** of his kingdom, and enjoy a **peaceful old age**.

Problems

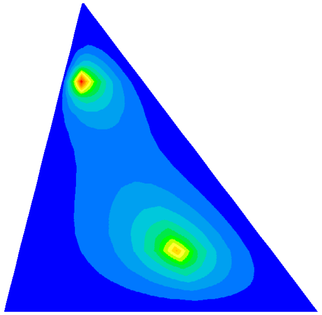
His **daughters** made the play truly into a tragedy.

Progress

BUT.... maps **are** used with success by **2D-population modellers** of combustion and **might** be **by swirl-flow** modellers also.

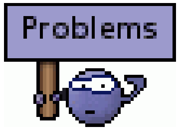


The turbulent-combustion map-users

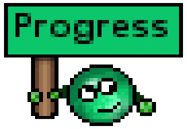


The population of turbulent reacting gases at a space-time location can be described by contours on a **temperature-rise *versus* fuel-air ratio** map.

THEN populational CFD can solve equations which, for each location, **compute population-member-concentration changes** resulting from **merging** and **differential convection.**



Well-tested formulations for differential convection are still lacking;

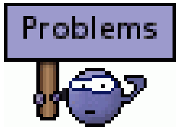


BUT... one can always guess;
or **neglect**!

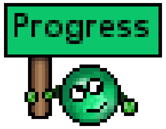
A turbulent-swirling-flow map

For swirling flows, **circumferential** velocity and **radial** velocity are plausible **map co-ordinates**.

THEN **equations** for particle movement through this 'population space', **based on momentum conservation,** could be solved,



Differential convection is of the essence; and the 'engulfment' process of population-member - merging must probably be replaced by another.



BUT... the turbulent-combustion **pattern** could be used as a start.

End of Part 1
Beginning of Part 2

Here ends the 25-century revew

Now follows a closer look at turbulent-combustion models from the populational view-point

Contents

2.1 Describing further the **Tri-Mix 'map'** of turbulent combustion..

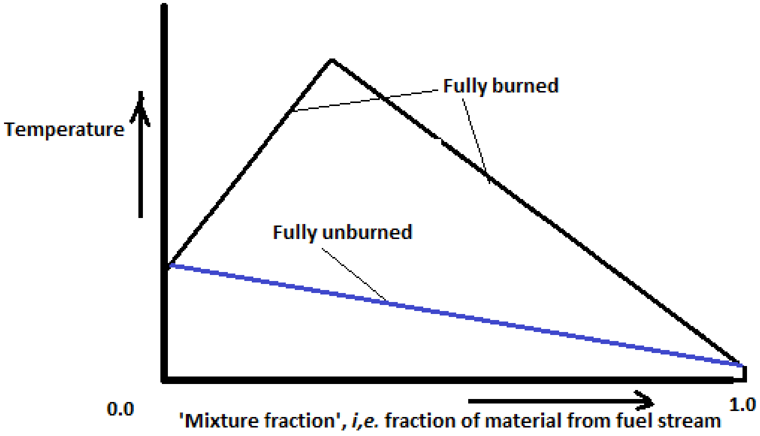
2.2. **Placing** models of turbulent combustion **on the map.**

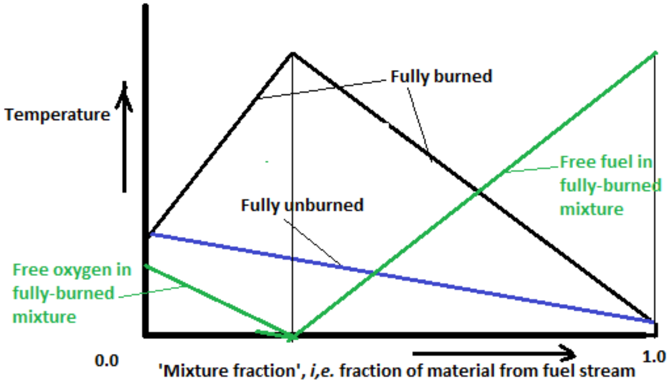
2.3 Explaining how gas-state distributions can be computed *via* **finite-volume equations**

2.1 The Tri-Mix map;
Well-known precursor plots.

The right–hand plot shows how the **temperature** of a fuel-air mixture varies with fuel proportion, when fuel is (upper) fully **burned** and (lower) fully **un-burned**.

The '**adiabatic temperature rise**' is the vertical distance **between** them.





The left-hand plot shows the **free-fuel** and **free-oxygen** values for the fully-burned condition,.

The mixture fraction at which both oxygen and fuel are zero is called '**stoichiometric**'.

The 'TriMix' diagram is a way of mapping the states which lie <u>between</u> the fully-burned and fully-unburned extremes.

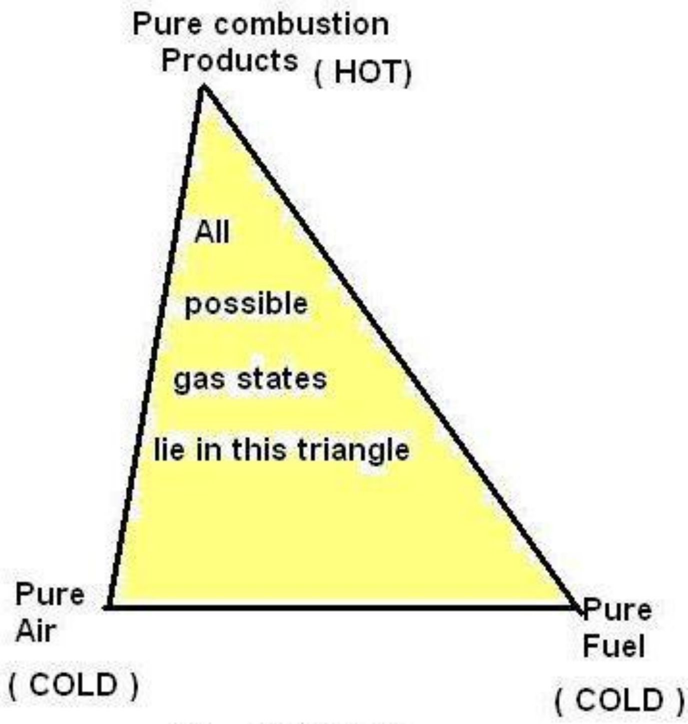
The Tri-Mix map; uses, and nature

The diagram con be used:

- for **describing** fuel+air flames; and
- for representing and comparing **theoretical models** of combustion.

Its **horizontal dimension** is mass fraction of fuel-derived material, or, **in atomic_nitrogen terms**:
1.0 - atomic_nitrogen fraction/0.768.

Its **vertical dimension** is the **adiabatic temperature rise** resulting from complete combustion of the fuel
(to CO2 and H20).

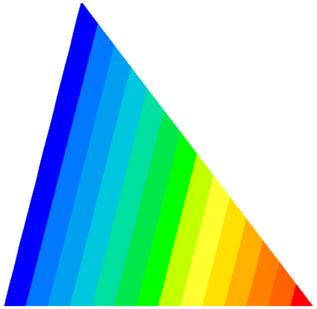


The TRIMIX diagram
(i.e. Temperature Rise~MIXture fraction)

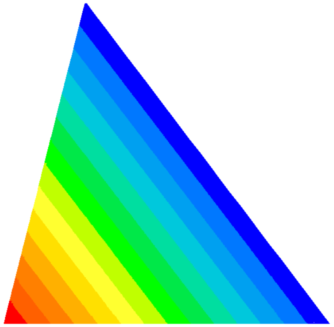
Points lying outside the triangle correspond to **non-physical negative concentrations**.

The Tri-Mix map; contours of various thermo-physical attributes

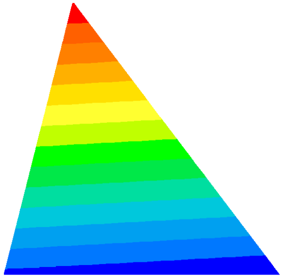
If we assume that diffusivities of all gases are equal, C and H oxidise in proportion, and concentrations of O, OH, NO, *etc* small, then:

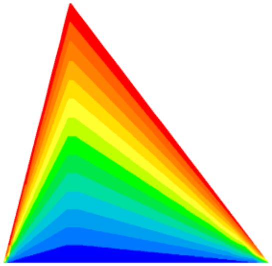


here are the distributions of unburned **fuel** (left) and free **oxygen** (right). Red is high, blue low, in all cases.



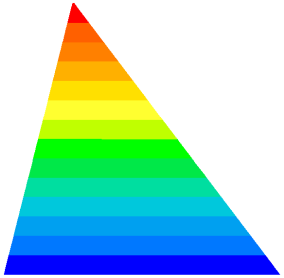
Here is the (adiabatic) gas **temperature** (right);





and the **reactedness** (left);

and finally the concentration of **combustion products** (right).

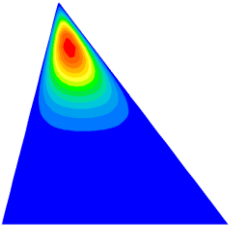


Any other properties such as density and viscosity can also be computed and displayed.

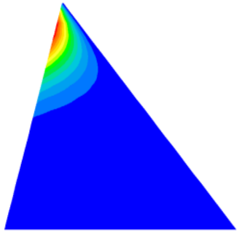
The Tri-Mix map; contours of various chemical reaction rates

Knowing the composition and the temperature, chemical kineticists can (in principle) compute the instantaneous **rates of chemical reaction** per unit mass of mixture in the various states.

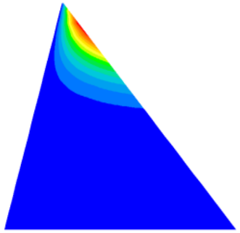
There are **three kinds** of reaction to be considered, of which the **rate-contours** are shown below (red is high rate; blue is low rate):



1. the main **energy-producing oxidation** of the fuel, which is what we **desire** to promote;



2. the **undesired** reaction producing **oxides of nitrogen**; and



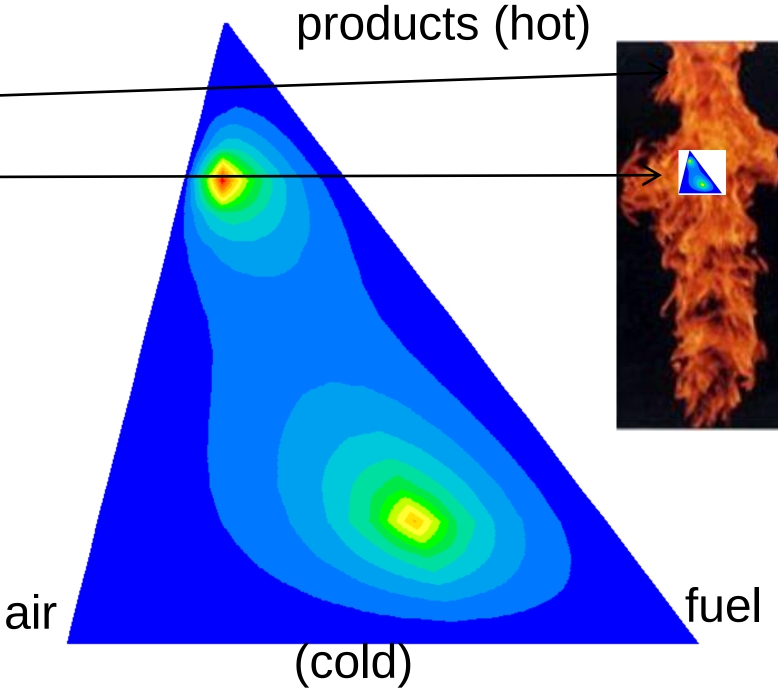
3. the often equally-undesired **smoke-creating** reaction.

4.. Note that we have not yet consideried any particular flame
We have simply assembled knowledge about the attributes of **all possible members** of the gases-in-flame population.

The Tri-Mix map; contours of population-member density

This contour diagram **does** relate to a **particular flame**, and to a **particular geometric** location. It describes **the proportions of time** in which the gas at that point is in each of the possible **states represented on the state-map**.

Time proportion means **probability** or **mass fraction** or **population density**. Multiplication by their reaction rates & integration over the triangle gives **total** rates of heat, NOX & smoke formation.



The **task of simulation** of turbulent combustion is therefore 'simply' that of determining **what this population-density distribution actually is**.

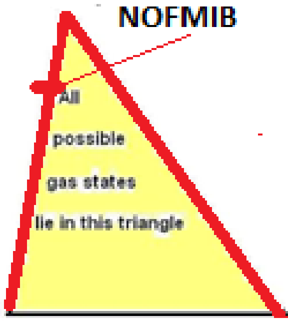
Of course, this must be done for **every location** in space; and, for non-steady flames, for **each (**not too small**) instant** of **time**; or rather, for **each 'cell**' in the **space-time** grid of the computation.

2.2 Putting models on the map; two **one-member** populations

Modeling means ‘**neglecting awkward facts**’ such as:

- diffusion coefficients **do differ somewhat** from gas to gas; and
- oxidation of the C and H in a hydrocarbon **do not** proceed at **always-proportionate** rates.

These neglects are not too far from the truth..



Very far is the **often-used NOFMIB model** (*i.e.* **NO-Fluctuations, Mixed-Is-Burned).**

Its ‘population’ is a **single point** on the **upper boundary** of the triangle.

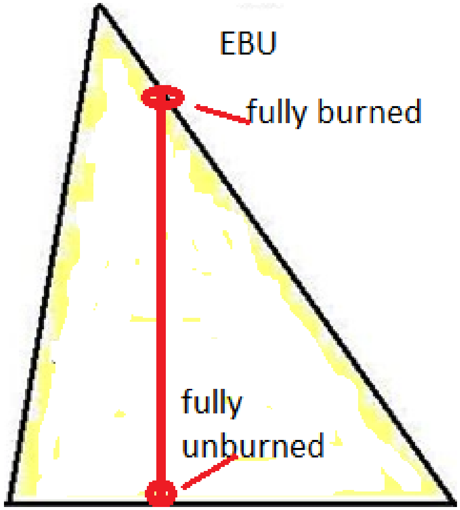
The horizontal position is determined by solving a **single** finite-volume equation for the **mixture fraction.**

Little less extreme is **NOFL** (*i.e.* **NO-FL**uctuations), which also uses **single-point** representation, but does allow the point to be **anywhere** in the triangle.

Two finite-volume equations determine its location: for **mixture fraction** and for **unburned-fuel** fraction.

Models on the map:
two-member populations

The **eddy-break-up** model(1971) postulated a population of **two members,** both having the same **fuel ratio**, but **one fully burned** & the other **fully unburned.**



The two members were supposed to **collide**, at rates fixed by **hydrodynamic** turbulence, forming **intermediate**-temperature and -composition material which **quickly** became fully burned.

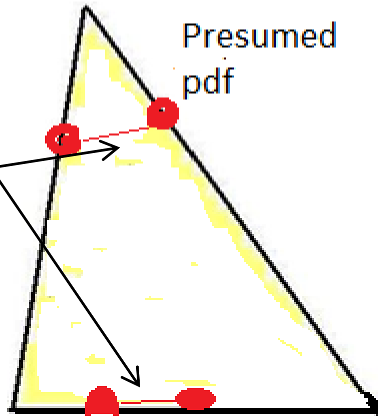
This model provided a (negative) source term in the finite-volume equation for the unburned fuel fraction, often expressed as:

$$-\ \mathbf{constant} * \mathbf{density} * r * (1 - r) * \varepsilon / k$$

where *r* is the local reactedness of the mixture, so that $r : (1-r)$ is the ratio of burned to unburned material; **ε & k** are from k-epsilon model.

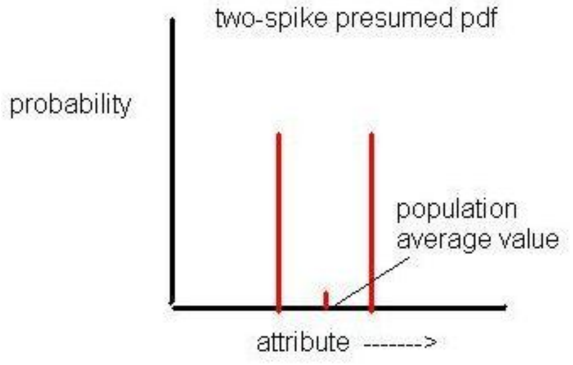
This link between **hydrodynamics** and **reaction rate** appears in some form, in almost all subsequent models of combustion.

Models on the map
the 2-member presumed-pdf model



Also in 1971 appeared the first **‘presumed-pdf**’ model, which is represented by the two red blobs on the base. (because at first the fluids were non-burning), and by two more on the sides when extended to **mixed-is-burned** models of turbulent flames**.**

Their locations were computed from **two** finite-volume equations: for the **mixture fraction** and for the **root-mean-square fluctuations**.
The second of these (the ‘***g***-equation’) was **novel**.



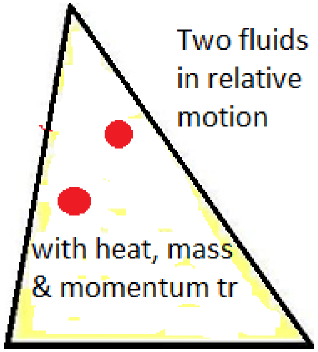
The presumed shape of the pdf *(i.e*. probability-density function) is shown on the left*.*

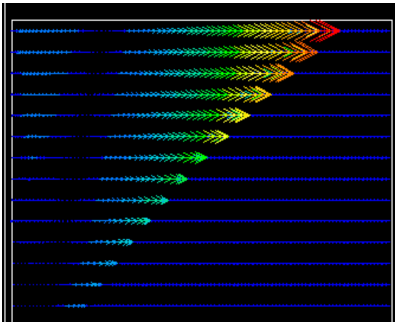
Variants of this model are still often used.

Another 2-member model on the map
two-Navier-Stokes-equations model

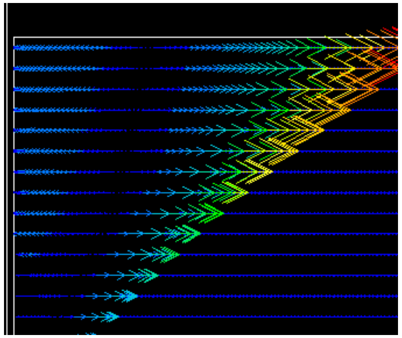
Invented so as to **simulate two-phase *(e.g.* steam-water) flows, the IPSA algorithm** was applied in 1982 to **a two-member** population of burning gases.

It solves mass, momentum and energy **equations for both** members; predicts their **relative motion**.





In flames propagating in ducts, **hotter** members (right) overtake **colder** ones (left); so mixing and combustion are intensified.
[Time is UP; distance RIGHT]



This model **can accommodate** and generalise **EBU, EDC** (see later slide) and **presumed–pdf** assumptions. But it is seldom used. **Why not?** Few professors have paid attenion to two-phase-flow CFD.

A pity; for this model **can** do what **conventional** turbulence models can**not**: namely **simulate un-mixing**.

Models on the map:
A four-member-population model

Melbourne
2011

Ninth Australian Heat and Mass
Transfer Conference 2011

Two facts about turbulent pre-mixed flames in plane-walled ducts

1. Increasing flow velocity increases flame speed; flame angle is constant

2. Sufficient increase of velocity **extinguishes** the flame

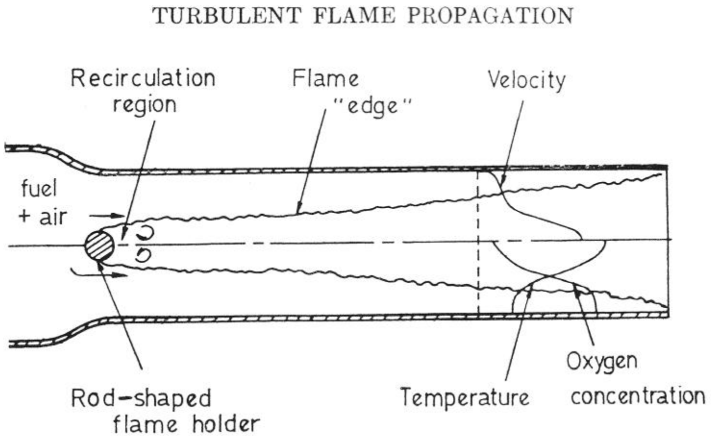
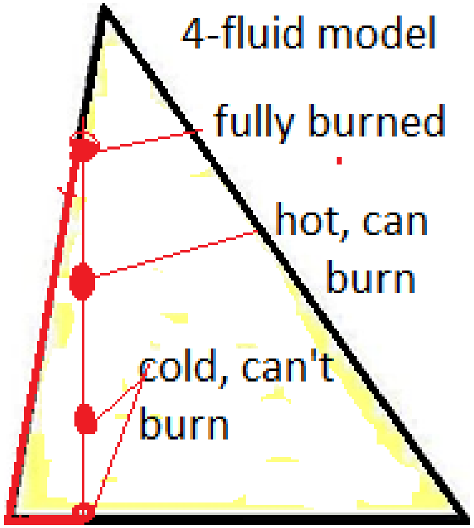


FIG. 1. The process under consideration.

EBU (2-fluid) explained 1, not 2.



The solution (24 years later !) refine the 'population grid'.

Eddy-break-up used a **two**-member population; so why not try using **four?** It **worked!**

The presence of the '**hot, can burn**' fluid (see left) allows space for chemical kinetics.

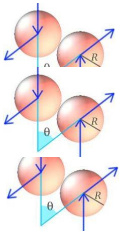
So extinction could be predicted (in principle).

How the four-fluid model allowed for finite chemical reaction rates

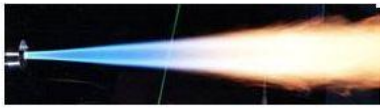
The Eddy-Break-Up postulate was that fully-burned and fully-unburned gas fragments **collided** and merged, at concentration-proportional rates, and the resulting mixture combusted instantly. With 4 fluids, there are **more pairings** possible.

<u>Collisions</u> between fluids

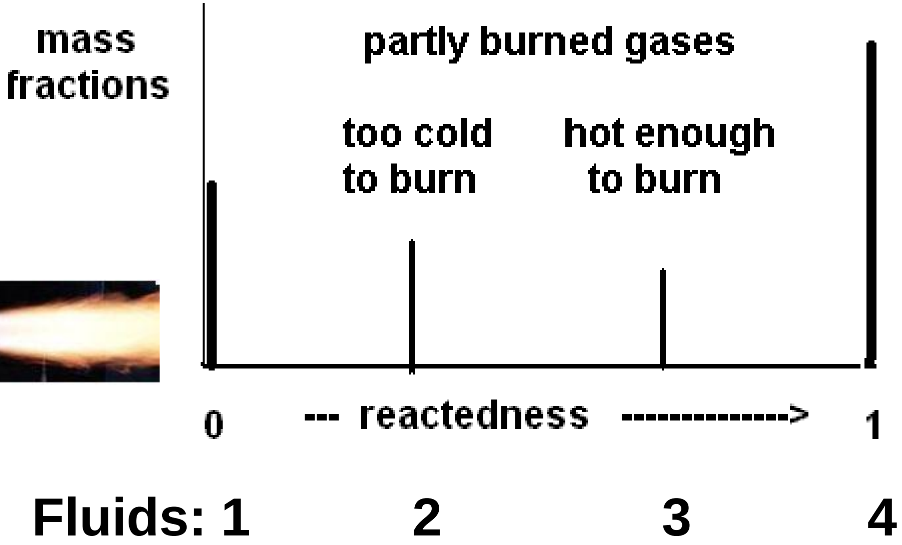
1 and 3 created fluid 2,
2 and 4 created fluid 3,
1 and 4 created fluid 2
and also fluid 3.



<u>Reaction</u> of fluid 3
created fluid 4
at a **chemistry-controlled** rate..



profile presumption of the four-fluid model



Applications of the four-fluid model to transient pre-mixed flames

The four-fluid model was **used successfully** for simulating flame spread in a **baffled duct** and for **oil-platform explosion** simulation.

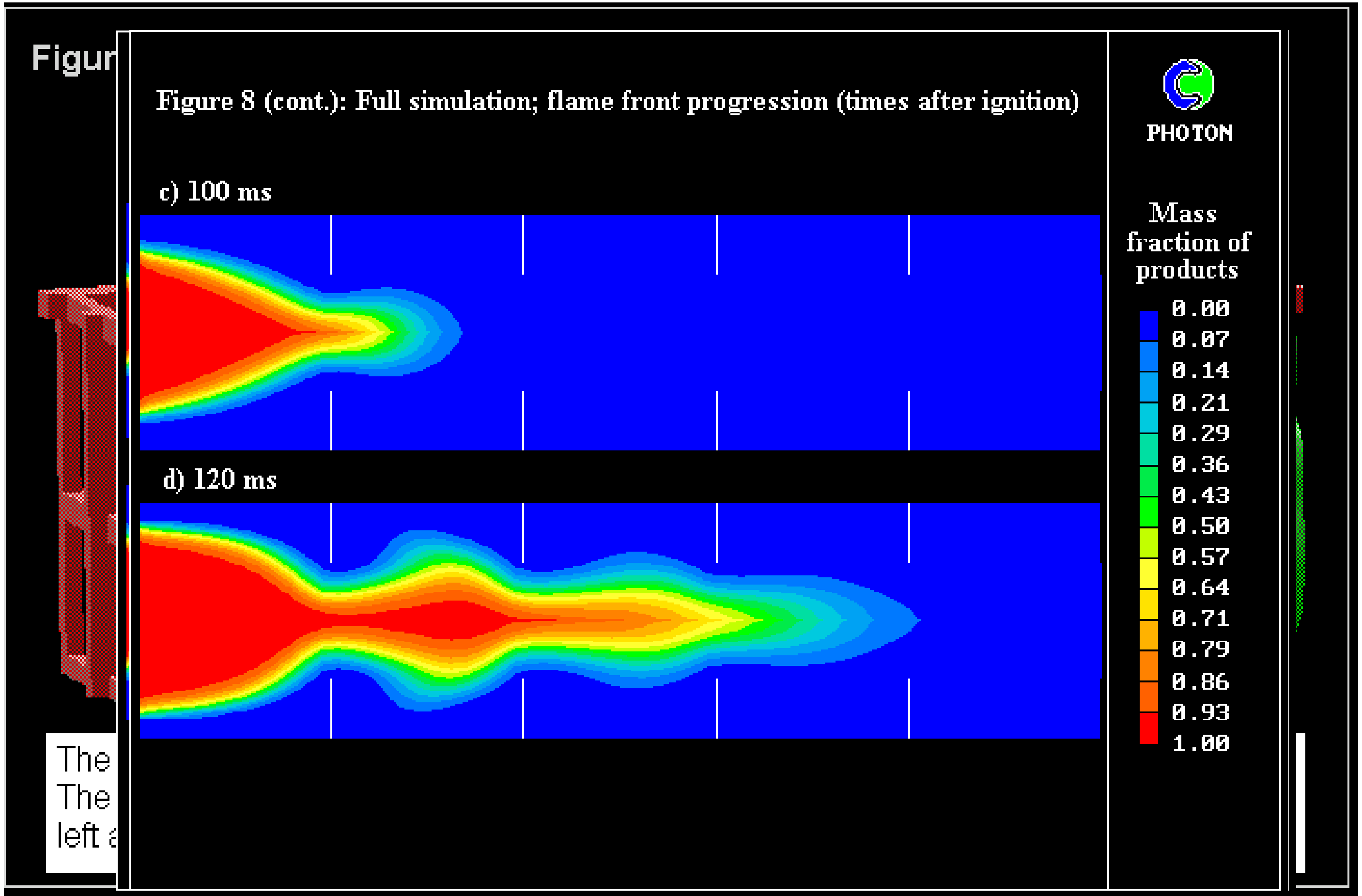
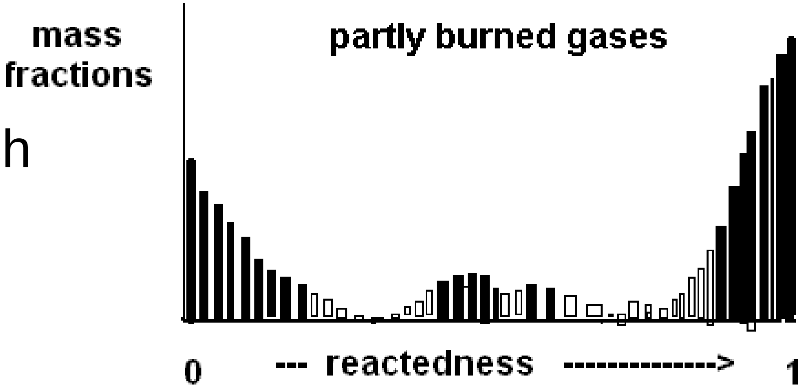


Figure 8 (cont.): Full simulation; flame front progression (times after ignition)

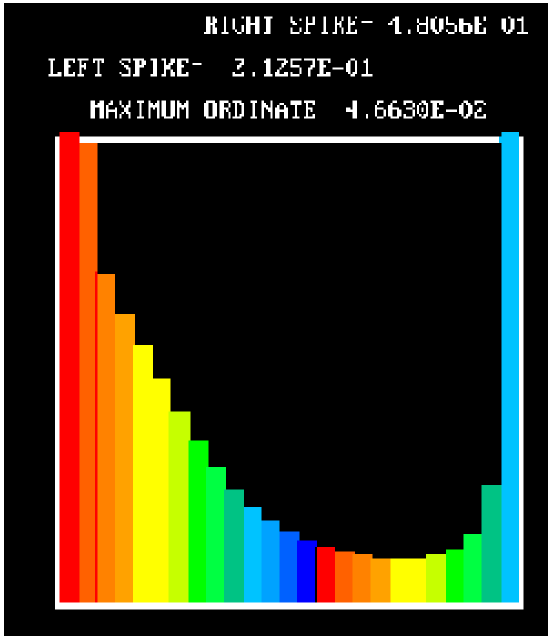
Models on the map:
from 4 to many; **the multi-fluid model**

In conventional CFD, we **divide space-time** into as many intervals as accuracy requires.

profile presumption of the MULTI-fluid model



Why not do the same for the population-defining variable at each point? **This worked too!**



On the left is the calculated pdf of a 40-member population in a ‘well-stirred reactor’.

Its shape depends in the relative rates of **merging** and reaction and on the postulated dependence of the latter on **reactedness**..

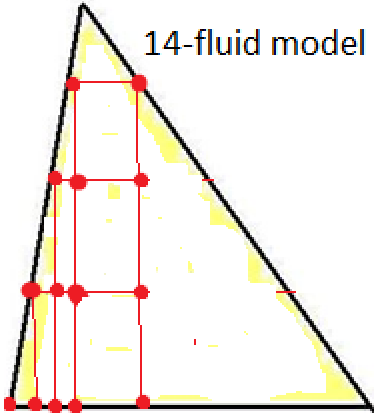
The (truncated) spikes at left and explain the success of the EBU **spikes-only** presumption.

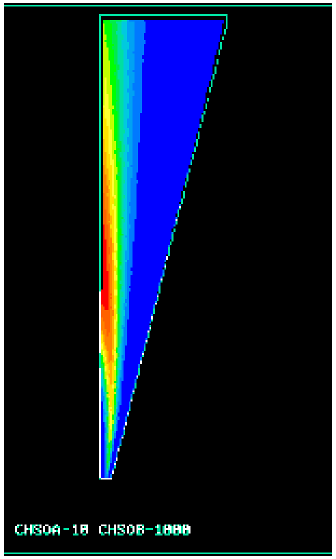
Models on the map :
A fourteen-member 2D population

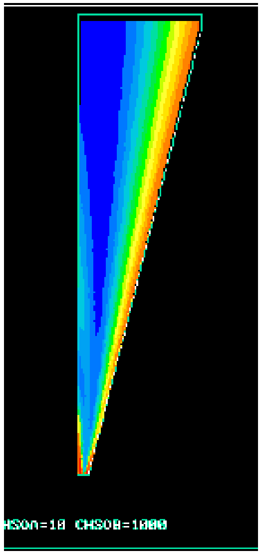
Melbourne
2011

Ninth Australian Heat and Mass
Transfer Conference 2011

EBU **is** often applied to non-premixed flames, with dubious validity.
So a 1996 **fourteen-fluid model** was the partly-pre-mixed Bunsen-burner flame.
Its TriMix representation is shown on the right.

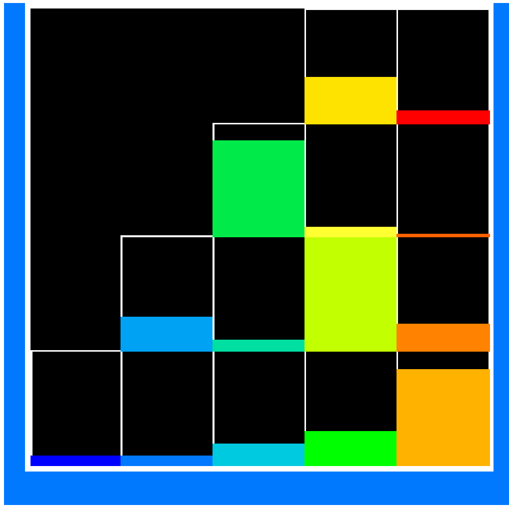




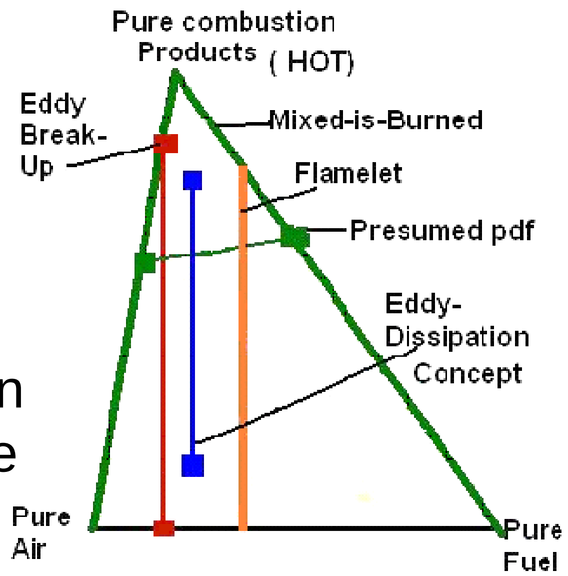


On the left are concentration contours of two of the fluids for a turbulent Bunsen burner.

On the right is a 2D probability density function for one point in the flame. (Trimix had not yet been invented).



Other models on the map:
1. eddy-dissipation concept ; 2. flamelet



1. The 1981 EDC postulates a two-member population; its members are (1) the so-called '**fine structures**', occupying little space; and (2) the **remainder;** both are shown as blue blobs on the right.

It is claimed that the fine-structures location allows the reaction rate of the mixture to be calculated. What a **clever blob**!

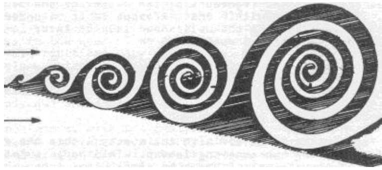
2. The 1980 **Flamelet** model postulates a population **distributed** along a vertiical line, from unburned to burned, but (like EBU) with most fluid at the ends.

The shape of the distribution is supposed to be the same as in a steadily-propagating laminar pre-mixed flame. But why should it be?

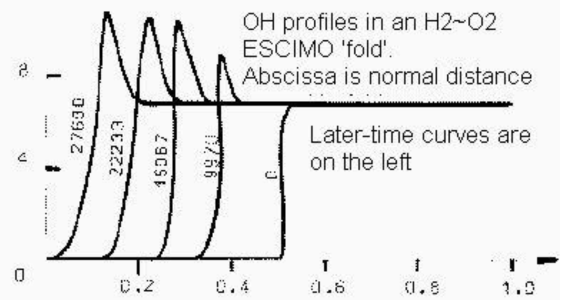
The last assumption allowed complex chemical kinetics to be introduced, and much computer time to be consumed. But their **dubious basis** renders their results correspondingly doubtful.

Other models on the map: 3. **ESCIMO (=Engulfment, Stretching, Coherence, Inter-diffusion , Moving Observer)**

The 1976 ESCIMO model also saw small laminar flames as players in turbulent combustion, namely as (more plausible?) **rolling-up vortices**.



These were subjected to one-dimensional unsteady analysis with results as indicated.

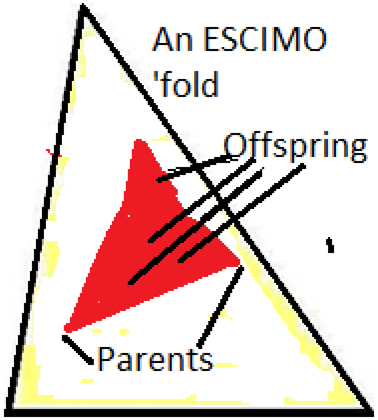


OH profiles in an H2~O2 ESCIMO 'fold'.
Abscissa is normal distance

Later-time curves are on the left

In contrast to ''flamelets', the 'engulfed' and 'engulfing' parents of a 'fold' could have **any temperature and composition.**

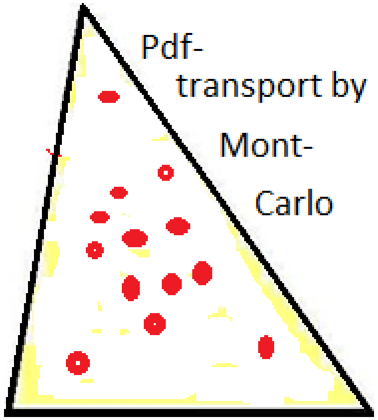
Therefore an 'ESCIMO event' might have been represented on the TriMix diagram by way of a patch as shown on the right.



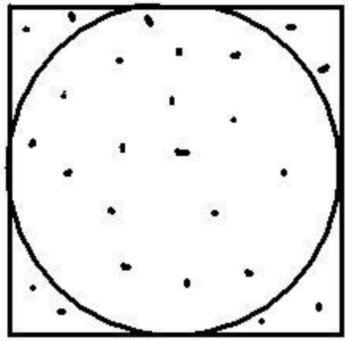
ESCIMO was 'in **advance of its time**'; but its ideas may yet come to fruition as part of populational CFD.

Other models on the map:
4. **the ‘Pdf-Transport’ Model**

Populations can be completely described in **terms** of **probability-density functions**; so the 1981 ‘pdf-transport model’ **appeared** to meet the need.



Unfortunately, its first introducer chose the **Monte Carlo** method for solving the transport equations, expressed on Tri-Mix as random points.



This is **legitimate**, just as one **can** compute π by counting how many uniformly sprinkled sand particles lie **inside** and how many **outside** the circle. But there are quicker ways!

Therefore large computing times, and foreign-to-CFD-specialist language, have delayed development of the model.

Why is Monte Carlo still used? Look left.

2.3 How population distributions can be best computed

Currently fashionable models of combustion (EBU, EDC, flamelet) and turbulence (RANS, LES**) lack essential populational** ingredients.

Pdf-transport is weighed down by its **Monte Carlo** baggage and unlike-CFD jargon.

But **discretized-population CFD** is as **easy to use** as **conventional** CFD; it just has a **few extra items** namely:

- extra **variables**, *viz* mass fractions of each population element;
- extra **terms** in *equations* , *viz.* **merging**; **differential convection**
- extra **empirical constants** , *e.g.* for **merging_rate / (ε/k)**
- extra **research** opportunities , *e.g.* unstructured **population grids**
- extra **avenues to explore** , *e.g.* **population-grid** refinement
- extra **experimentally-testable ite**ms, *e.g.* population-member **concentrations** and attributes

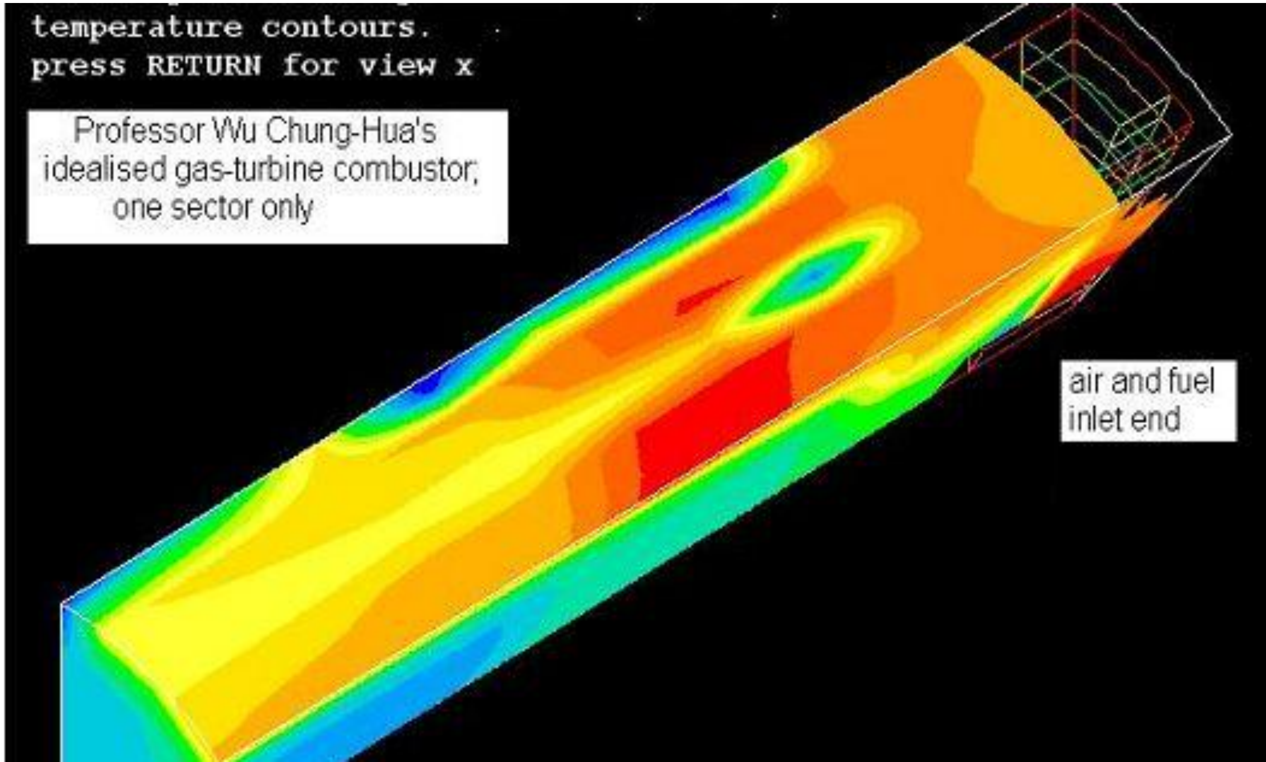
Alexander Pope wrote: ”Be not the first by which the new are tried.”

Don’t worry. You **won’t** be the first.

Populational CFD is not all that new.

Here is a 30-year old calculation of temperature contours in (one sector of) an idealised gas-turbine combustor,

NOFL was the model used



```
temperature contours.
press RETURN for view x
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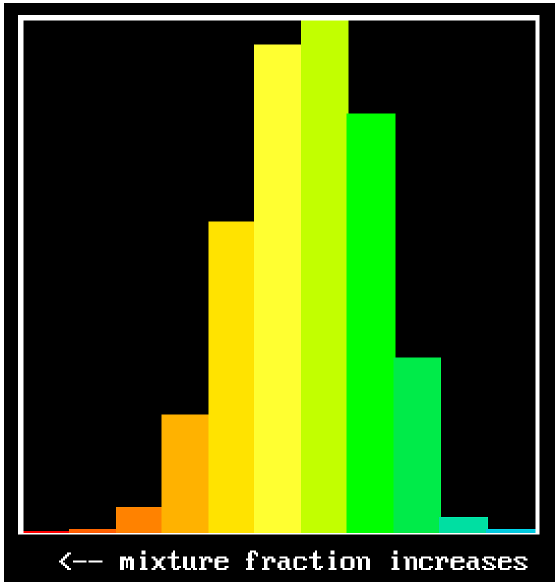
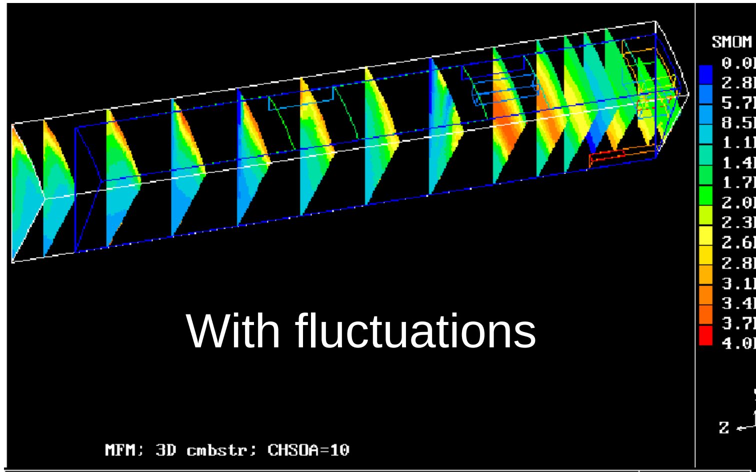
Smoke formation rate is influenced by turbulent fluctuations

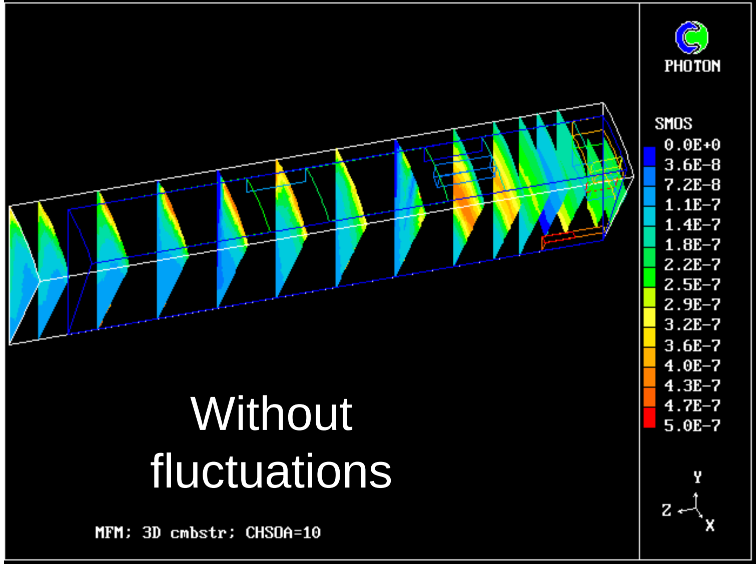
20 years later, this combustor was used to show how **fluctuations** of fuel-air ratio affect predictions of rates of **smoke formation.**

The small **differences** are **significant** when CFD is being used to **optimise the design**.



A 10-fluid model was used with fuel-air-ratio as the population-dimension Each cell had its own pdf.





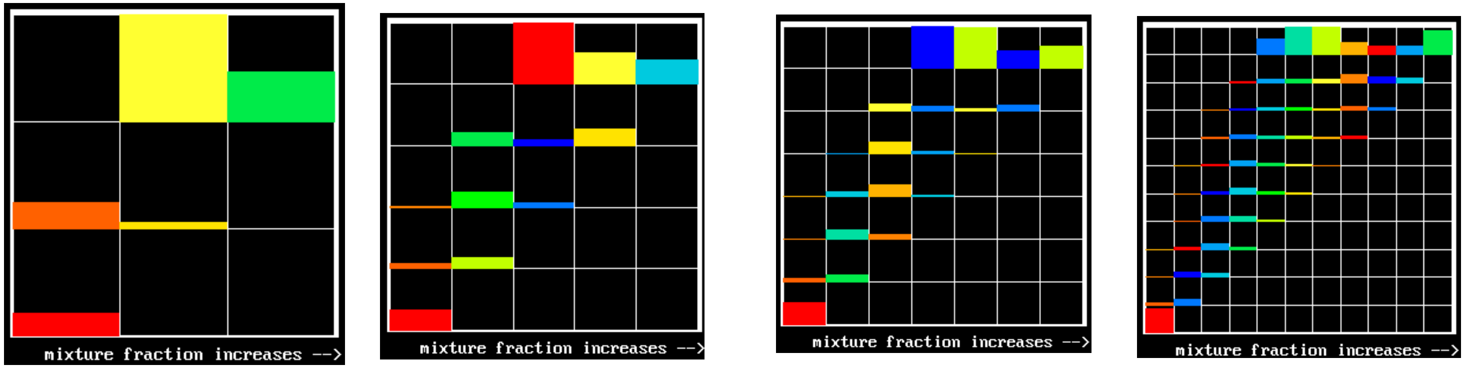
Computing population distributions;
a grid-refinement study

2-, 4-, 14-, 40-, 100- and multi-member populations appear above. But **how many** does one truly need? There is no **general** answer.

In **conventional** CFD, the needed sizes of **space interval** or **time step** are found by comparing results obtained with **various** sizes .

The same is true of **Populational** CFD. **Grid-refinement** studies must be made, as shown here for a 2D population:

Four pdfs for the same geometric location with population grids:

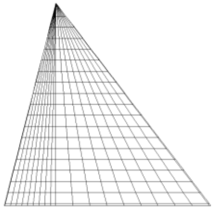


3*3 5*5 7*7 11*11

The Monte-Carlo approach **lacks** this grid-refinement capability.

Computing population distributions *via* **discretization of TriMix**

The TriMix plane can be discretised in various ways. The 2D pdf’s just seen used lines of **constant Temperature rise** and constant **Mixture fraction**; but **that left some cells empty**.



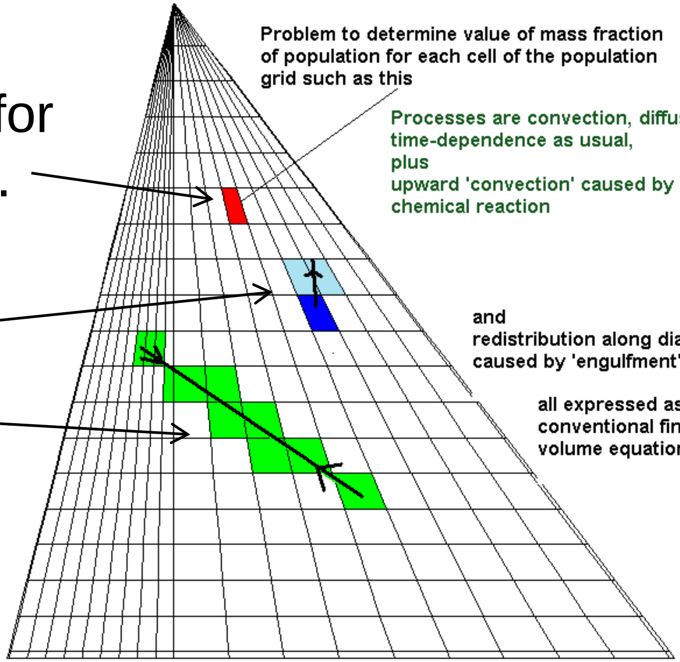
The grid shown on the left is better, using **constant reactedness lines** as the second co-ordinate.

Finite-volume equations are solved for the mass fraction of gas in each cell.

As well as convection and diffusion, these contain terms for reaction

and for engulfment.

The **engulfment-rate** formula can be that of EBU, until a better one is discovered.



Problem to determine value of mass fraction of population for each cell of the population grid such as this

Processes are convection, diffusion & time-dependence as usual, plus upward 'convection' caused by chemical reaction

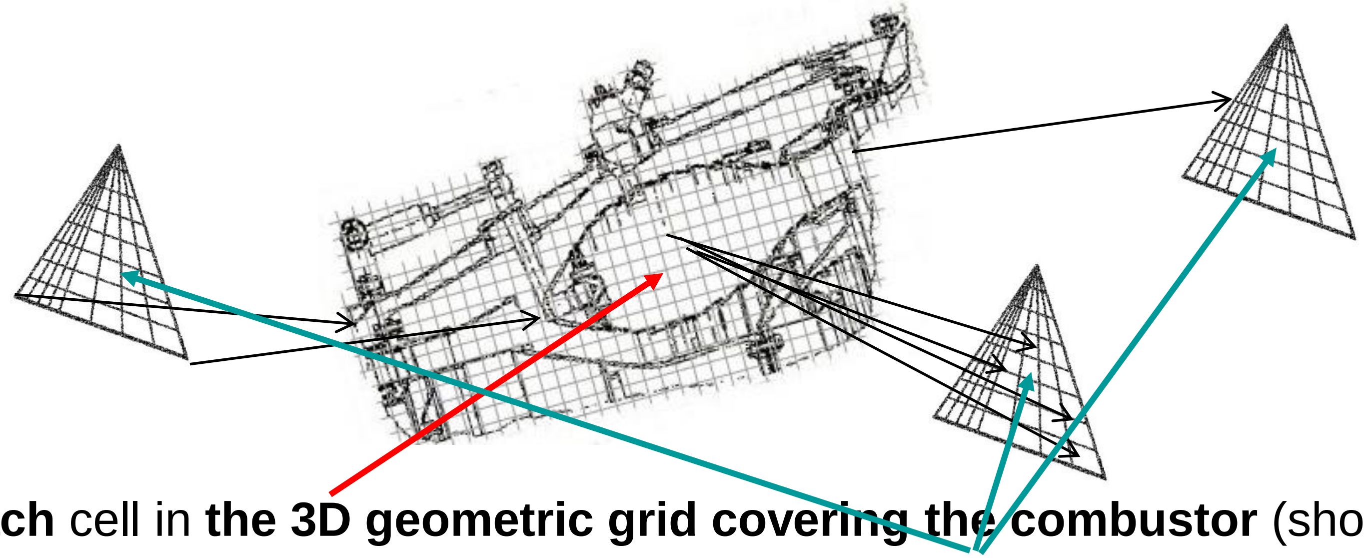
and redistribution along diagonals caused by 'engulfment'

all expressed as conventional finite-volume equations

Computing population distributions *via* TriMix, **for all space locations**

Melbourne
2011

Ninth Australian Heat and Mass
Transfer Conference 2011



For **each** cell in **the 3D geometric grid covering the combustor** (shown 2D here), there corresponds **one** set of cells in the **2D population grid**. So the problem might be thought of as **five-dimensional**.

That term is **too alarmist;** all that has happened is that the **3D problem** has acquired some **additional dependent variables**, equal in number to the cells in one 2D population grid, typically between 10 and 100.

Thus, **without** the population dimension, the dependent variables might have been p, u, v, w, ke, eps, f, T; and **with it** they become been p, u, v, w, ke, eps, f1, f2, f3, ... f20, say, **without immense** computer-time increase.

Concluding remarks,1

Populational CFD is ready for application to practical problems.

The prospects of realistic combustor modelling *via* the populational approach **are good**.

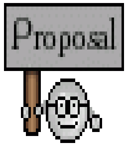
But they have been good for **fifteen** years! Yet resources are still being wasted on too-narrowly-conceived LES, EDC and flamelet models. Why? Too many MOTSmen (MOTS=More Of The Same)

Not enough POTSmen (POTS=POpulaTion Student

I hope to have shifted the balance today.

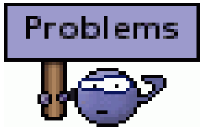
If only it were as easy as that!

Concluding remarks, 2
the future

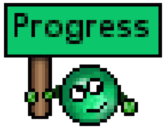


IF it is at last recognised that **‘More-Of-The-Same’** turbulence modelling is **hopeless**,

THEN, **switching attention** to populational modelling will make **improved predictive capability certain**.



Setbacks are also certain, and (hard-to-find) **resourcefulness** will be needed.



BUT… history shows that old ideas **always are** replaced by **new** ones.

So this slide marks **only** of **this** lecture,
not of continued progress, **the END.**