Turbulence and combustion;
a New State-Map,
by Brian Spalding

November 2010

Imperial College seminar

This lecture is about **turbulence** generally; but focuses on flames because their '**unmixedness'** is easy to see.

This diffusion flame shows **hotter** gases interspersed with **colder**; but in **non**-reacting fluids **faster**- and **slower-** moving intermingle likewise.

So turbulent fluids are best understood as **populations** consisting of: hotter/colder, faster/slower, richer /poorer, younger/older *etc*. members.

Turbulence models **neglecting** population aspects are **not realistic.**

Attributes of populations; dimensionality

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- **We choose how** to distinguish **human-**population members : *e.g. by* height, weight, wealth, age, skin-colour, *etc.*
- We often **discretise** population dimensions: *e.g.* In terms of 'age-groups', 'income-brackets', *etc.*
- **Different** choices are made by: tailors, nurses, tax-inspectors, insurance agents *etc*. Choice depends on **purpose**.
- The population-**average** value of height, weight, temperature, *etc.* Is seldom as interesting as their **distributions** within the population..
- **Heat-transfer** specialists may choose **temperature**, because radiation depends on its fourth power.
- **Combustion** specialists need to consider temperature **and** fuel-air ratio; for each influences chemical-reaction rate.
- Each attribute can be regard as a **dimension;** so heat transfer analysis requires a **1-**, and combustion a **2-**dimensional population.

A state-map for turbulent combustion: its many uses

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Maps are two-dimensional, and combusting gases create a two-dimensional population of gas states; so a **combustion state-map** can be created. It has many uses, namely:

- Combustion chambers are devices which cause gases to change their state, *i.e*. their positions on the map**.** **Designers** can use the map so as to find the **best route.**

- **Theories** of combustion are numerous; and differences of nomenclature obscure both differences and similarities. Placing them on a **common map** clarifies both.

- If X-land has good maps ,Y-land's cartographers may be inspired to improve their own**. Combustion's** example could be followed for - **swirling flow**; **gusty winds**; **air pollution; chemical reactors**; and many more subjects.

A state-map for turbulent combustion: outline of the lecture

This lecture has four parts, namely:

1. Introduction, now concluded.
2. Description of the Tri-Mix ‘map’ of turbulent combustion.
3. Review of models of turbulent combustion, including placing them on the map.
4. Describing how gas-state distributions can be computed *via* discretisation.

Although the ‘map’ aspect of the lecture is novel, much of its content is several decades old, albeit not yet exploited,

Despite its industrial importance and scientific interest, progress in this area of science is deplorably slow.

Part 2. The Tri-Mix map; Precursor plots.

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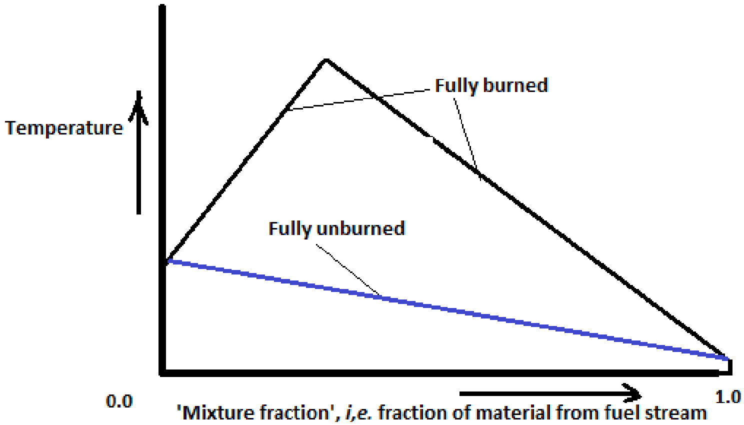
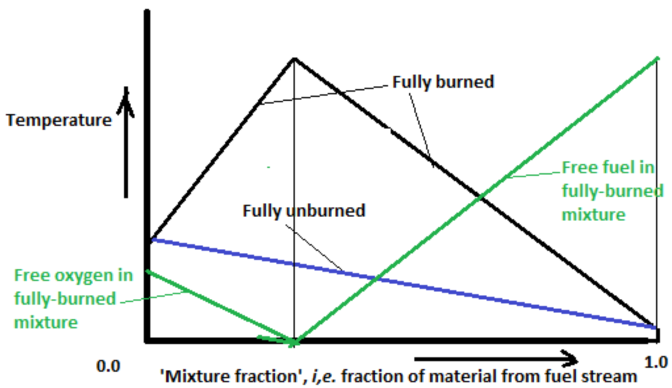
The familiar plot on the right shows how the **temperature** of a fuel-air mixture varies with the fuel proportion, when the fuel is (a) fully **burned** and (b) fully **un-burned**.
The '**adiabatic temperature rise**' is the vertical distance between them.





The plot on the left shows the **free-fuel** and **free-oxygen** values for the fully-burned condition,.
It is also very well-known.
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 between** the fully-burned and fully-unburned extremes.

The Tri-Mix map; an introduction

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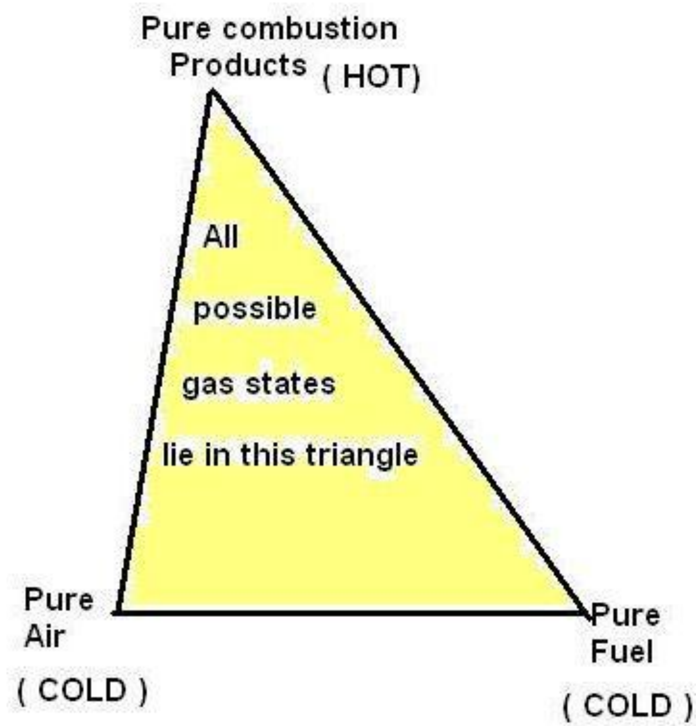
Here is the diagram which I shall use as **a ‘state-map’**:
• for **describing** fuel+air flames;
• for planning ‘**design journeys**’; and
• for representing and comparing **theoretical models** of combustion.



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

Its **horizontal dimension** is mass fraction of fuel-derived material, or, **in atomic 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).

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

The Tri-Mix map; contours of various thermodynamical attributes

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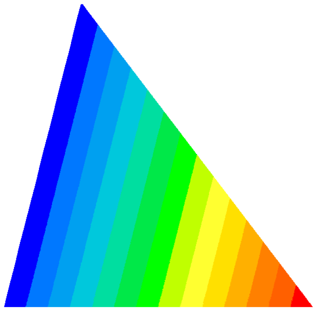
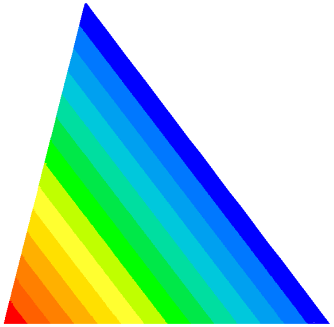
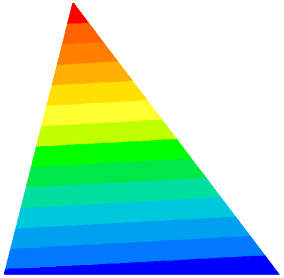
If we assume that: diffusivities of all gases are equal, C and H oxidise in proportion, and concentrations of O, OH, NO, *etc* small, then:

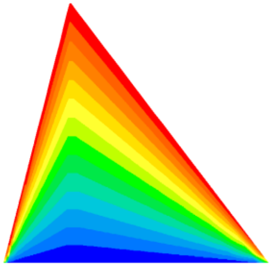


here are the distributions of unburned **fuel** (left) and free **oxygen** (right). Red is high, blue low, in all cases.



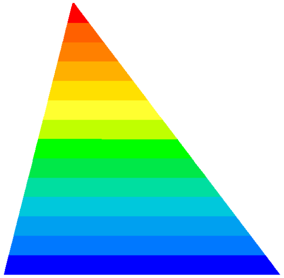
Here is the (adiabatic) gas **temperature** (right);





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

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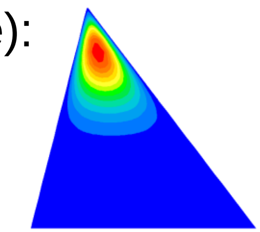
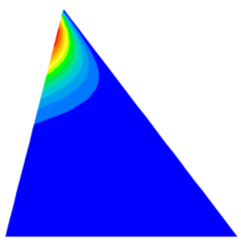
Knowing the composition and the temperature, chemical kineticists can (in principle) compute for us the instantaneous **rates of chemical reaction** per unit mass of mixture in the various states.

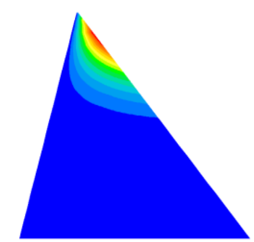
There are **three kinds** of reaction to be considered, of which the **rate-contours** are shown below (red is high rate; blue is low rate):

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 are not yet considering any particular flame
We are simply assembling knowledge about the attributes of **all possible members** of the gases-in flame population.

The Tri-Mix map; contours of population density

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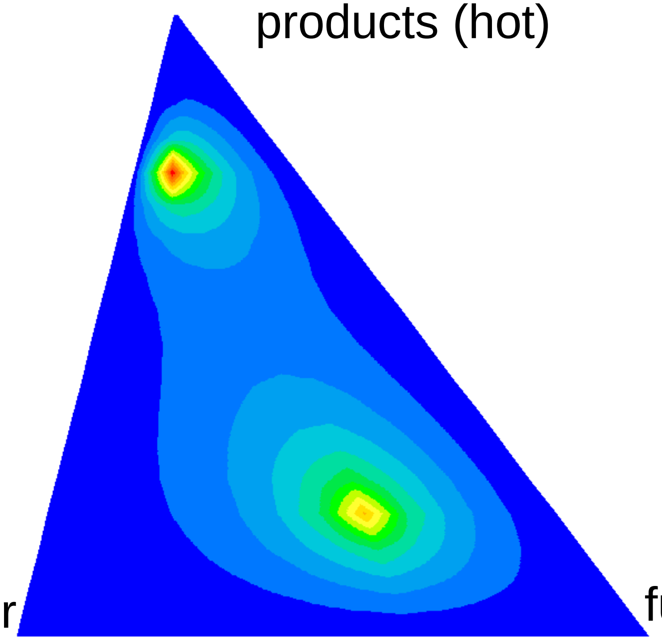
This contour diagram **does** relate to a **particular flame**; and to a **particular geometric** location**.** It describes **the proportions of time** in which the gas at that point is in each of the possible **states represented on the state-map**.

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.

The Tri-Mix map; designing a combustor means “planning a journey” “

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They should avoid the NOX and smoke-generation regions here:

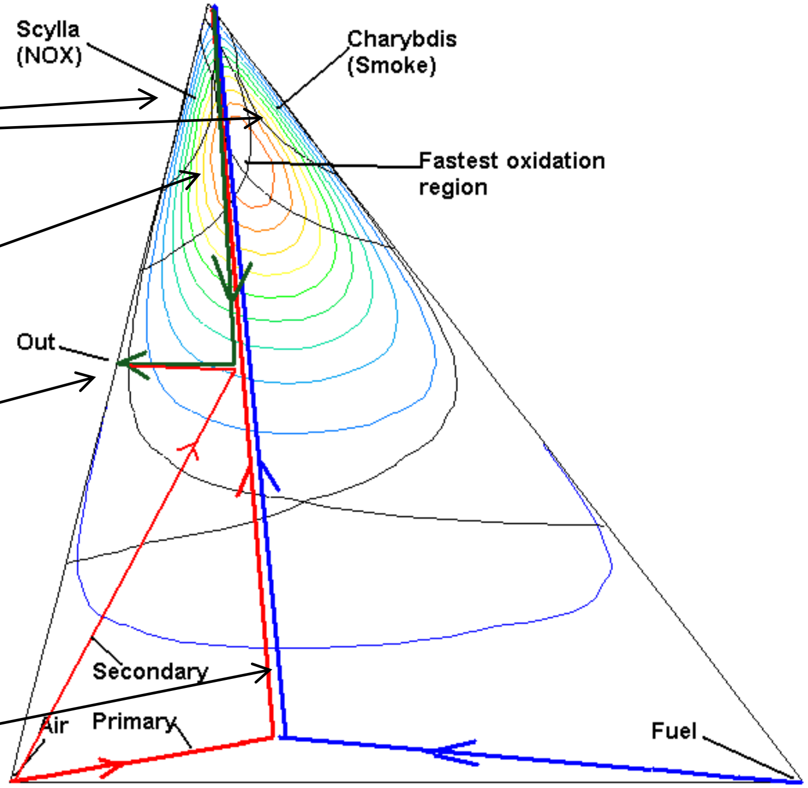
They should mix with hot product to reach the high-oxidation-rate region here:

Their journey, after dilution and cooling by secondary air, ends here:

The designer now knows how to achieve his ends.

Therefore they should mix stoichiometrically here:

A gas-turbine combustion chamber converts fuel and oxygen into CO_2 and H_2O.



Their journey starts here and here;

The Tri-Mix map; **how can one** compute distributions of population density?

To a modern CFD specialist the answer is obvious *viz*. 'in the same way as we compute distributions in **space & time** dimensions'.

Which is? To **discretise** the relevant dimension; to formulate **finite-volume** equations; and to solve these by **iterative** successive-substitution methods.

Forty years ago, the then-modern combustion specialists **thought differently**; and their thoughts, alas, still prevail.

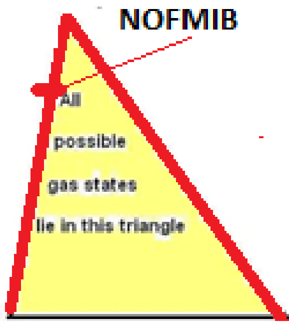
What is our task? To understand. Even to sympathise. And praise. But then to **pursue the modern way**.

I shall describe the 'modern way' in Part 4 below. But first, in Part 3, I discuss what has been happening in the last four (yes, four!) decades.

We therefore now begin to discuss '**Models of Turbulent Combustion'.**

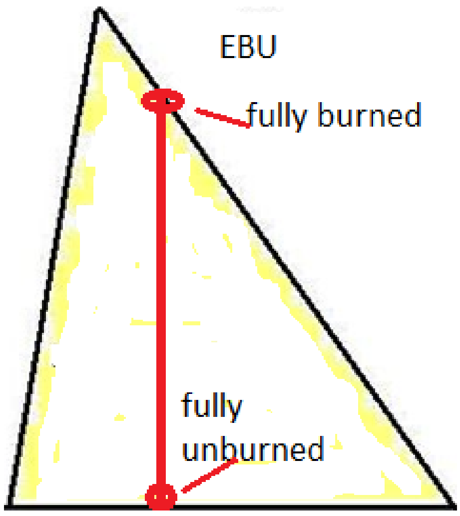
Modeling often means '**neglecting awkward facts**' such as:
• that diffusion coefficients **do differ somewhat** from gas to gas; and
• that oxidation of the C and H in a hydrocarbon proceed at **not always proportionate** rates.
These neglects are comparatively innocent.

At the other extreme is the **NOFMIB** (*i.e.* no-fluctuations, mixed-is-burned) **model,** which is **often used**
This represents the populationas a **single point** which must lie on the **upper boundary** of the triangle.
The location of that boundary is determined by solving a **single** finite-volume equation for the **mixture fraction.**



Little less extreme is **NOFL** (*i.e.* no-fluctuations), 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.

The first (1971) turbulence model to allow for fluctuations was **EBU** (*i.e.* eddy-break-up). It postulated a population of **two members,** both having the **same mixture fraction**, 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 itself fully burned.

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

$$- constant * density * r * (1 – r) * \varepsilon / k$$

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 of Turbulent Combustion; **two-member** populations (continued); presumed-pdf

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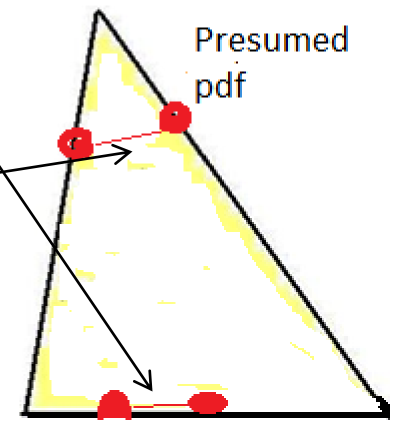
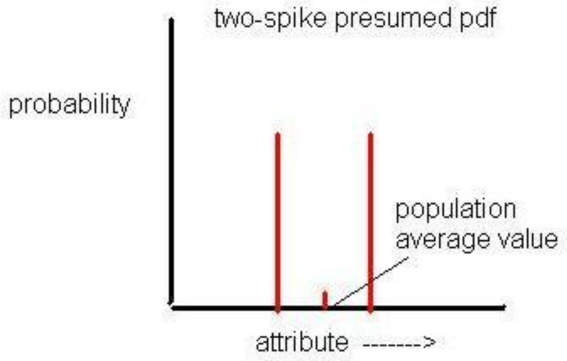
Also in 1971 appeared the first '**presumed-pdf**' model, which is represented by the two red blobs on the base. (because at first the fluids were non-burning), and by two more on the sides when extended to **mixed-is-burned** models of turbulent flames**.**



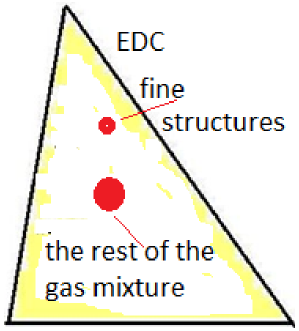
Their locations were computed from **two** finite-volume equations: for the **mixture fraction** and for the **root-mean-square fluctuations**.
The second of these (the '***g***-equation') was **novel**.



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

Variants of this model are still often used.

Models of Turbulent Combustion with two-member populations; the Eddy-Dissipation Concept



This model, purporting to account for finite chemical-reaction rates, appeared in 1981. Its two population members were so-called '**fine structures**', occupying little space; and the **remainder**. The former could be hotter than the latter, but had the same fuel-air ratio

The two members exchange heat and material at a rate determined by an EBU-like formula; but fine-structures volume fraction depends only on Reynolds number. The chemical reaction is supposed to take place in the fine structures only.

Its authors claim: *"The models presented here can readily handle complex chemistry and at the same time take care of turbulence interaction. Results obtained with these models are in close agreement with experimental data.*

Some CFD-code vendors believe them. Other, contrasting the extensive superstructure with the weak foundation, interpret the ED in EDC as: "Extremely Doubtful".

Models of Turbulent Combustion with two-member populations; the Two-fluid Model

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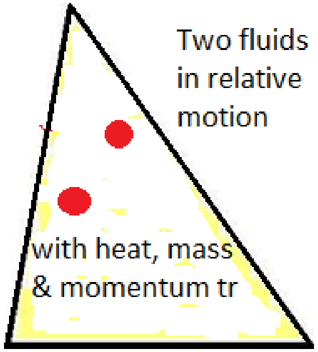
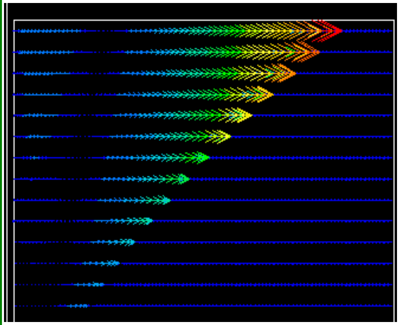
Invented so as to **simulate two-phase *(e.g.* steam-water) flows, the IPSA algorithm** was applied in 1982 to **a two-member** population of burning gases.

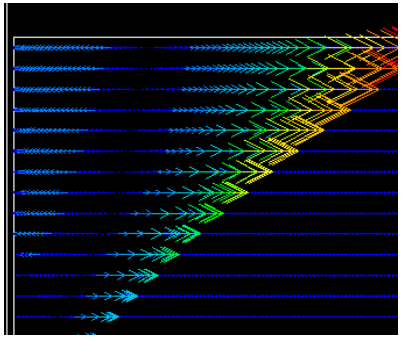


It solves **conservation equations for both** members; so they can **move** relative to each other.



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** and **presumed–pdf** assumptions. But it is seldom used. **Why not?**

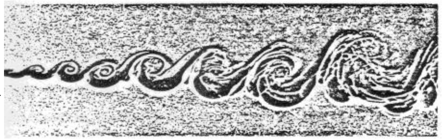
"It's not in Fluent, or Star-CD, or CFX. So it **can't exist**", some say.

'Two-member' is definitely better than '**one-member**', *i.e.* than neglecting fluctuations entirely.

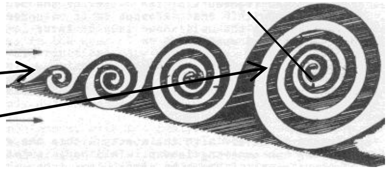
EBU's link to hydrodynamics was a lasting step forward.

Two-fluid provides a powerful means of **generalisation.**

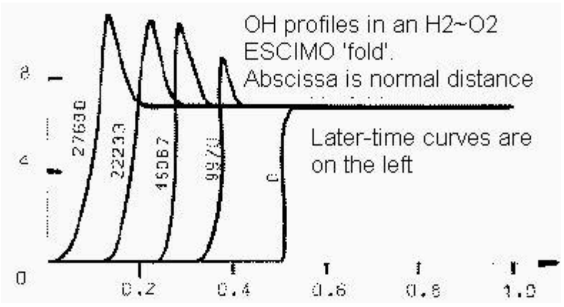
But two points are **not sufficient** to characterise **2D distributions**.



So a 1976 proposal imagined a turbulent fluid to consist of rolling-up vortices like this which could be idealised for numerical analysis thus



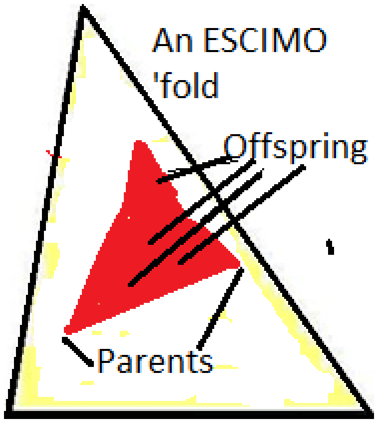
so as to compute **profiles** of temperature and concentration along lines normal to the 'folds', moving with the fluid, as shown here for OH in an H2~O2 flame. Complex kinetic schemes are easy to handle.



Models of Turbulent Combustion: **beyond** two-member populations; more about **ESCIMO**

ESCIMO stands for **En**gulfment, **S**tretching, **C**oherence, **I**nter-diffusion and **M**oving **O**bserver.

On Tri-Mix an engulfment event covers an area, '**parents**' being the engulfed gases which inter-diffuse and react to create '**offspring**' gases.



Since any two population members can engulf one another, the whole-population is represented by **super-position** of **patches**.

Three Imperial College PhD theses (Tam, Noseir, Sun) contain **biographical** ('fold') and **demographical** ('population') studies of this kind. However ESCIMO was '**in advance of its time**'.

Some of its elements can be discerned in the independently-developed (1980) '**laminar- flamelet**' model. This, because it passes the 'is-it-in-FLUENT?' test, has become popular as a name; but it appears as yet to have **no definitive formulation**.

Models of Turbulent Combustion:
beyond two-member populations;
the 'Pdf-Transport' Model

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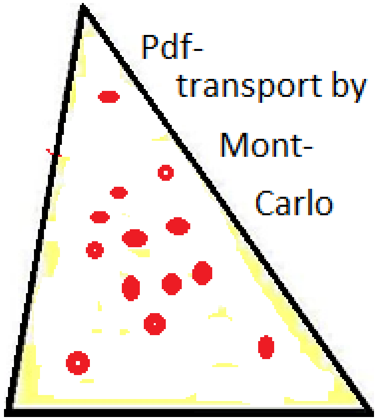
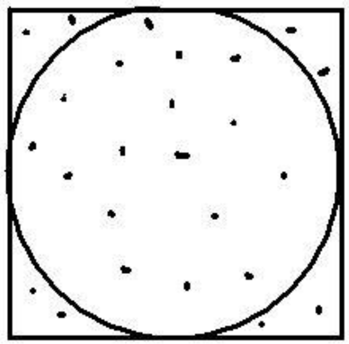
Since populations can be completely described in **terms** of **probability-density functions**, the 1981 'pdf-transport model' appeared to meet the need.

Unfortunately, its first introducer needlessly 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.

Part 4. Computing population distributions *via* **discretization; first steps.**

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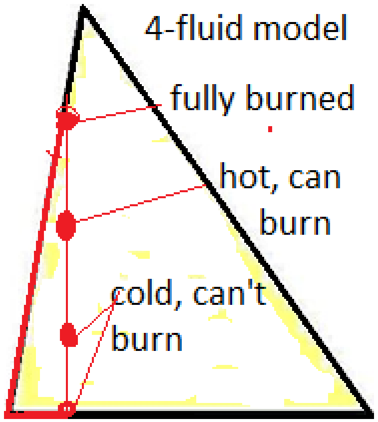
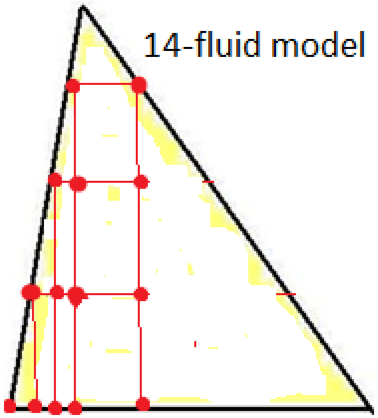
The four-fluid model of 1995 '**refined the grid**' of the Eddy-Break-Up model, namely from 2 to 4.

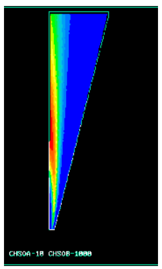


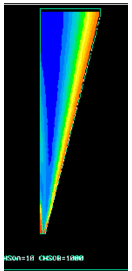
The four red blobs show the states of the four fluids all having the same air-fuel ratio.

This allowed chemical kinetics play a part; so **flame extinction** could be simulated.

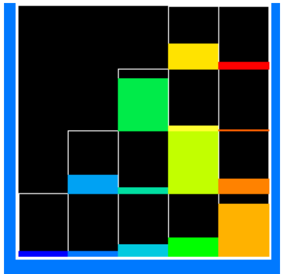
Although EBU is often applied to non-premixed flames, its validity is dubious. To fill this gap, in 1996 a **fourteen-fluid model** was created and applied to the partly-pre-mixed Bunsen-burner flame.
Its TriMix representation is shown on the right.







On the left are computed concentrations for two of the fluids.



Here is the 2D pdf for 1 point in space.

The obvious multi-fluid generalisation was swiftly made; but **too** swiftly to attract followers.

Therefore, to proceed more slowly now, I show slides from an earlier lecture

This starts with EBU and proceeds step-wise to MFM (multi-fluid model).

Confined pre-mixed flame; reactedness population

Scurlock's experiment

Pre-mixed fuel and air flow in steadily from left

Flame spreads from a gutter-shaped flame-holder in a duct with plane parallel walls. The velocity profile is shown.

I consider a flow in which the fuel and air are mixed **before** they enter, at uniform and constant velocity, a plane-walled duct in which is placed a **bluff-body 'flame- holder'**.

A turbulent **wedge-shaped flame** spreads across the duct, as the sketch indicates; and the profile of longitudinal velocity is roughly as shown.

What then limits **its** rate? **A different kind of mixing**: that between **burned and unburned gases.**

Confined pre-mixed flame; the near-constancy of its angle

When first investigated, this flame showed some **puzzling features**, namely that the **wedge angle** was **almost independent** of:

- inlet velocity
- fuel-air ratio;
- inlet temperature;
- pressure; and
- inlet turbulence intensity.

But **why?**

Confined pre-mixed flame; the first population presumption

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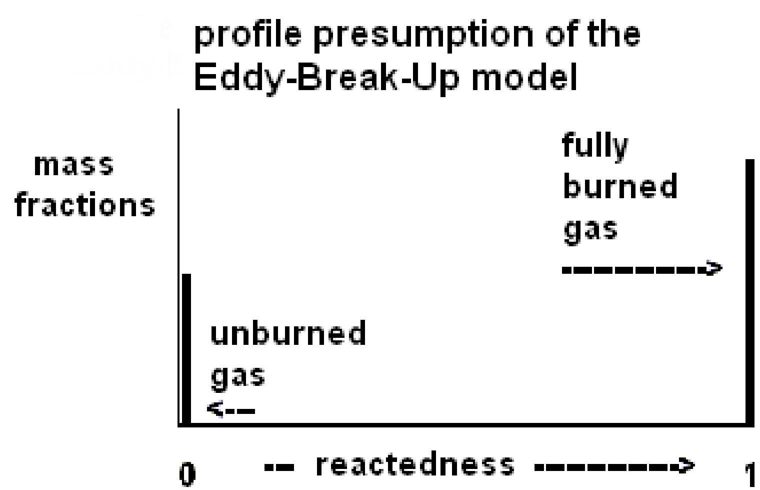
The guessed profile

The **first idea**, embodied in the so-called **eddy-break-up model ,** was that the gas population consisted **of two components**, namely:

(1) fragments of **wholly un-burned gas** which were **too cold to burn**; and

(2) fragments of hot **wholly-burned gas** which **also could not burn** because either all the fuel or all the oxygen **had been consumed**.

The **histogram** representing the **presumed** population therefore consisted of **two spikes**; and their relative heights dictated what would be measured as the **time-average temperature.**



Confined pre-mixed flame;
collision between burned and unburned gas fragments

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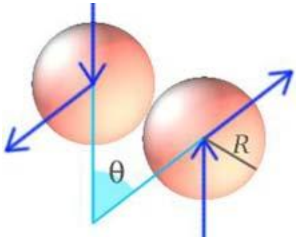


These two elements of the population were thought of as **colliding** with one another and thereby producing **sub-fragments** of intermediate temperature and composition.

These latter, being **sufficiently hot** and also **containing reactants**, **could** burn; and did so very rapidly, thereby **increasing the height of the right-hand spike**. Their actual concentration was considered, implicitly, to be negligibly small.

The rate of collision per unit volume was **guessed** as proportional to the **rate of dissipation of turbulence energy**.

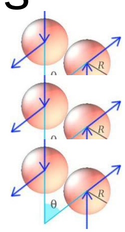
This explained why the flame angle remained almost unchanged when the inflow velocity was increased.

Confined pre-mixed flame;
the next presumed reactedness profile

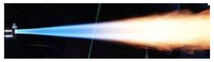
The four-fluid model

The EBU, published in 1970, became very popular; so much so that **25 years passed** before the obvious next step was taken;: to **increase the number** of presumed components **from 2 to 4** !

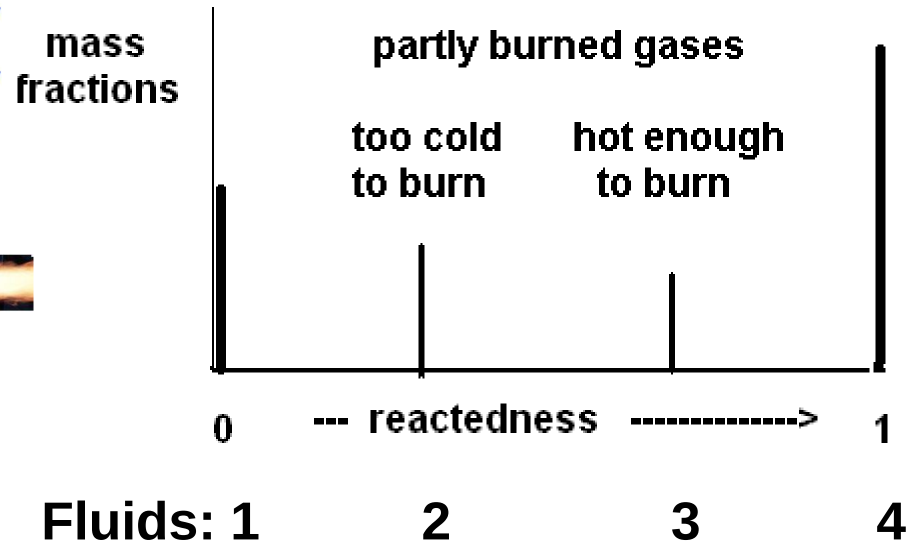
Collisions between fluids
1 and 3 created fluid 2,
2 and 4 created fluid 3,
1 and 4 created fluid 2
and also fluid 3.



Reaction of fluid 3
created fluid 4
at a **chemistry-controlled** rate.



profile presumption of the four-fluid model



Confined pre-mixed flame; applications of the four-fluid model

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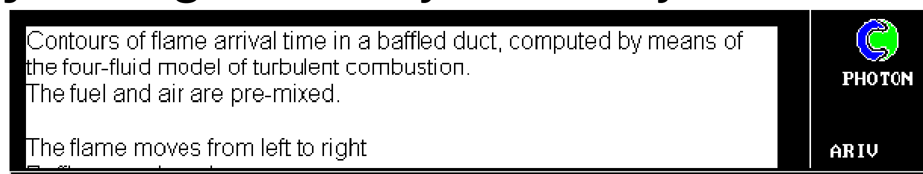
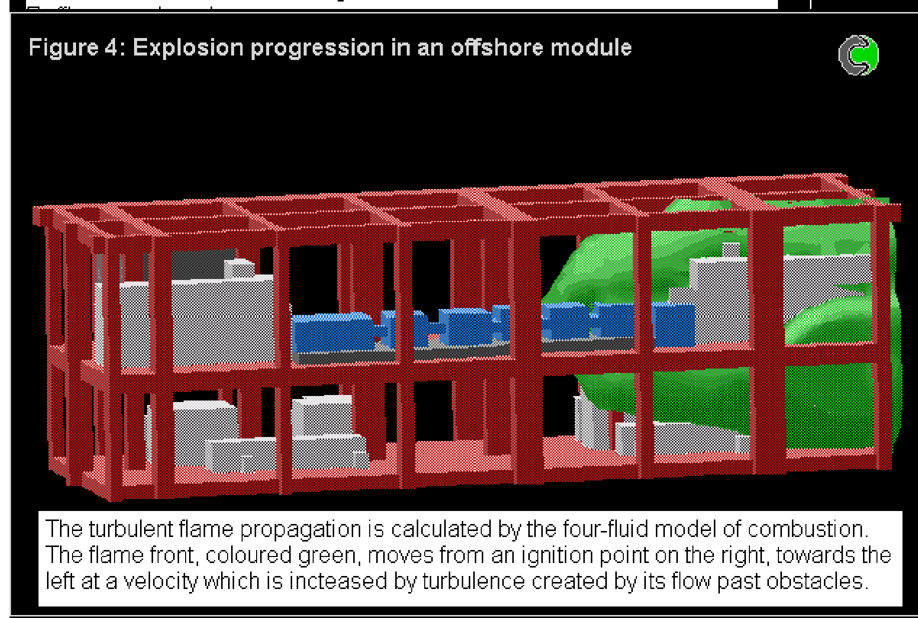
The **chemistry-controlled step** (fluid 3 creates fluid 4) **explained: why:**

1. the flame angle remained **nearly constant**, and
2. the flame could be **suddenly extinguished** by a velocity increase.

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

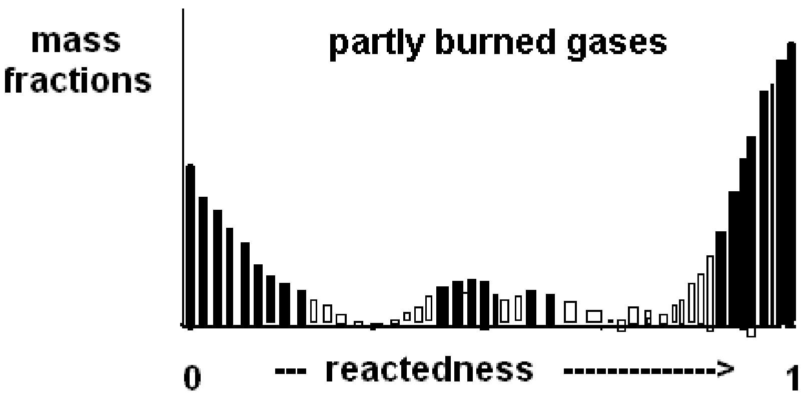
It has been little used; but it was the first step towards **calculating** the reactedness population.





From four fluids to many: the multi-fluid model

profile presumption of the MULTI-fluid model



In conventional CFD, we **divide space and time** into **as many intervals as we need.**

Why not do the same for the reactedness at each point?

The height of each column can then be deduced from a **Finite-Interval equation'** like this:

*height of interval= sum for all faces of coefficient * height of neighbour interval + sum of additional sources +* ***sum for all other intervals of coefficient * height of other interval)***

What the terms in the finite-interval equation represent

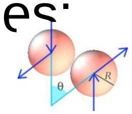
In: *height of interval= sum for **all faces** of **coefficient** * height of **neighbou**r interval +*

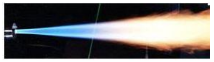
the **coefficient**s express rates of **convection and diffusion**, as in the the finite-volume equations of conventional CFD.

But in*: sum for **all other intervals** of **coefficient** * height of **other** interval*

the **coefficient**s express the **physical** and **chemica**l processes:

- **collision** between members of the fluid population, and
- **chemical conversion** of one member into another.





The **finite-interval method** is thus merely a **natural extension** of the **finite-volume method**; and its equations can be solved in the familiar successive-substitution manner

The calculation of population distributions is **easy**.

How material is distributed after collision

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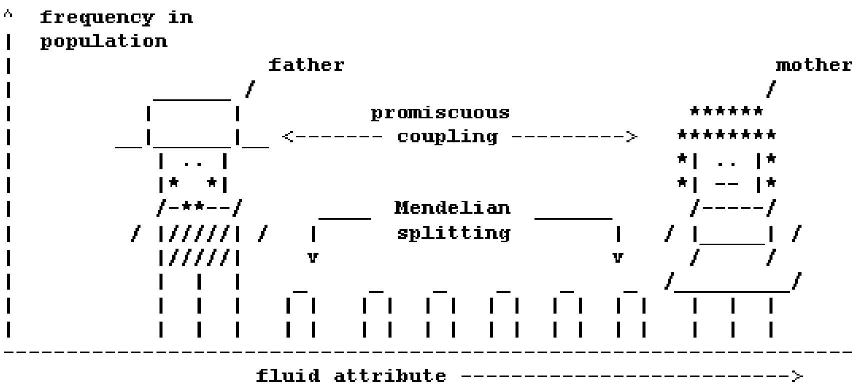
Here is a diagram from one of the earliest publications. It depicts one of the possible hypotheses, called '**Promiscuous Mendelian**'.



The **'colliders'** are treated as **'mother'** and **'father'**; and the word **'promiscous'** implies that **any two members** of the population may collide.

The word Mendelian, a reference to Gregor Mendel, the Austrian "father of modern genetics", implies that the offspring may appear with **equal probability in any interval between** those of the parents.

A calculated probability-density function

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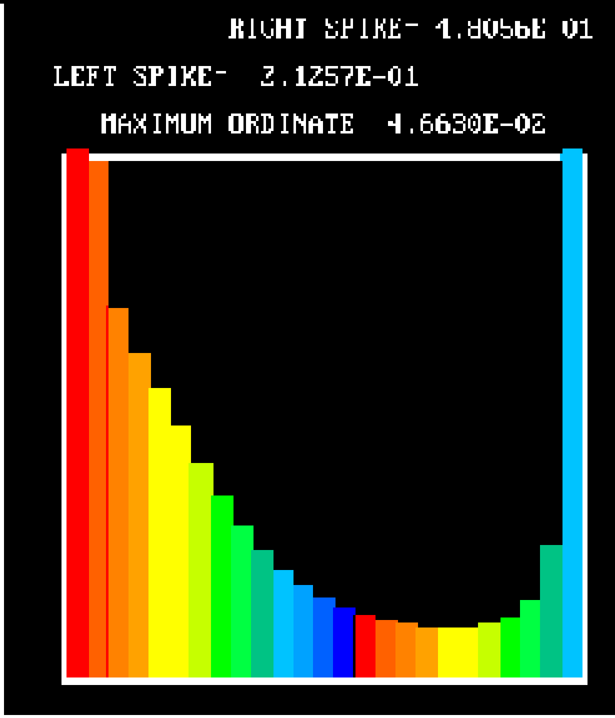
This hypothesis has been embodied in the PHOENICS computer code. Here is one **reactedness histogram,** computed with its aid.



As in the the eddy-break-up guess, there are indeed **spikes at zero and unity reactedness;**

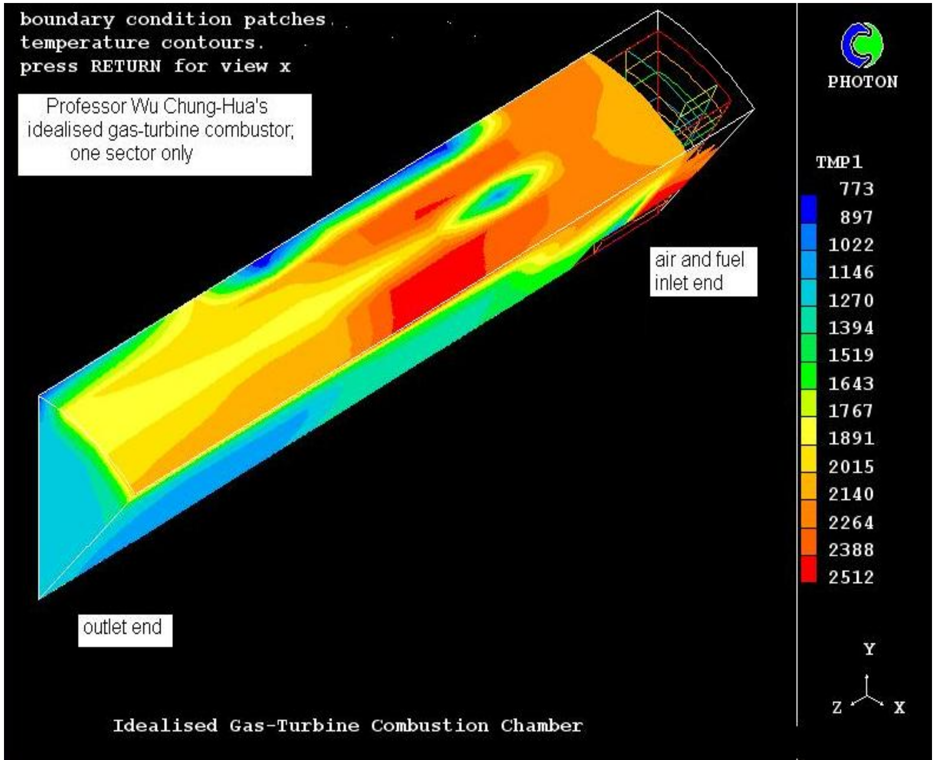
but calculation has shown that the intervals in-between are also populated.

Such probability distributions can to be computed **for each location** in the flame. Then the desired **reaction rate for the whole flame** can be deduced.

Application to gas-turbine combustion

A three-dimensional gaseous-fuel combustor

I show here one sector of a simple combustor proposed by Professor Wu Chung-Hua in the early days of PHOENICS.



Smoke formation rate is influenced by turbulent fluctuations

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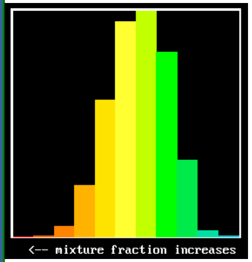
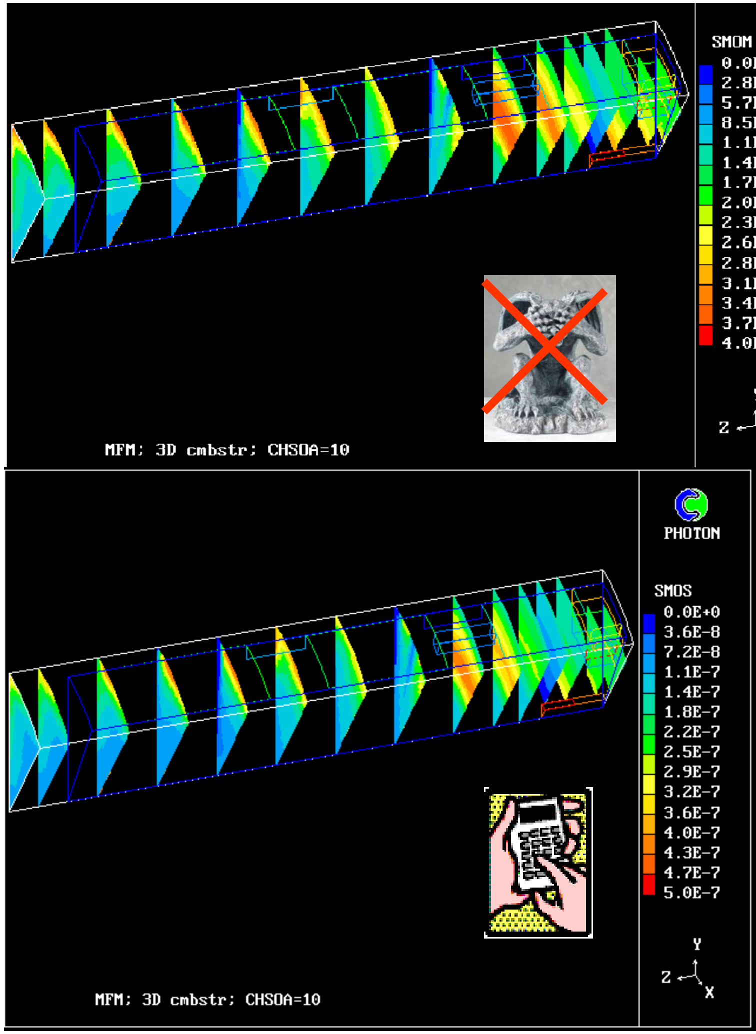
Much later, I used this combustor to show how **one must not neglect fluctuations** of fuel-air ratio when predicting **smoke** formation.



I used a 10-fluid model, with fuel-air-ratio as the population-defining attribute. Each cell had its own computed histogram

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



Part 4. Computing population distributions *via* **discretization;** the 2010 lecture continued

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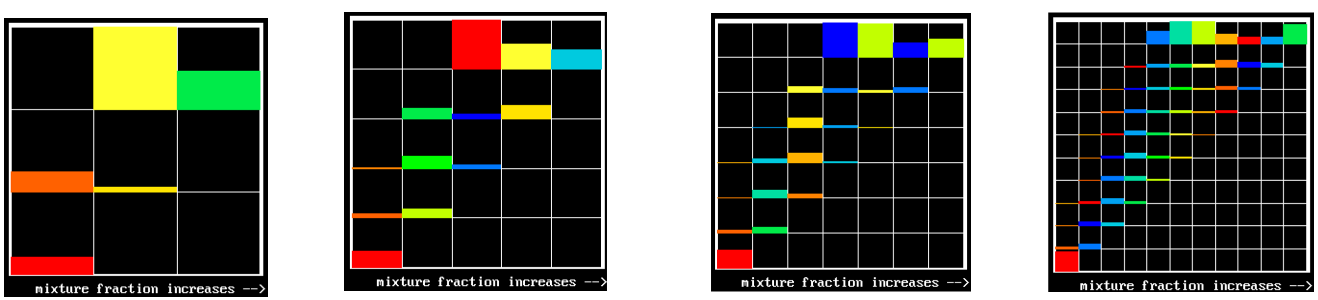
From the extract from earlier lecture we have seen how the 4-fluid model was used both in **applications** and as the starting point for **multi-fluid models**. The populations were **one-dimensional.**

Mention has been made of the early two-dimensional-population study, accessible from this link**,** of the turbulent Bunsen burner

Later studies explored the influence of 'population-grid refinement' on the accuracy of the results as illustrated below, where 3*3, 5*5, 7*7and 11*11 grids are compared for the same geometrical location in a flame.



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

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

November 2010

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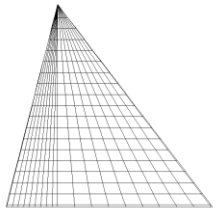
The TriMix plane can be discretised in various ways. The 2D pdf's just seen used lines of **constant Temperature rise** and constant **Mixture fraction**; but that left some cells empty.



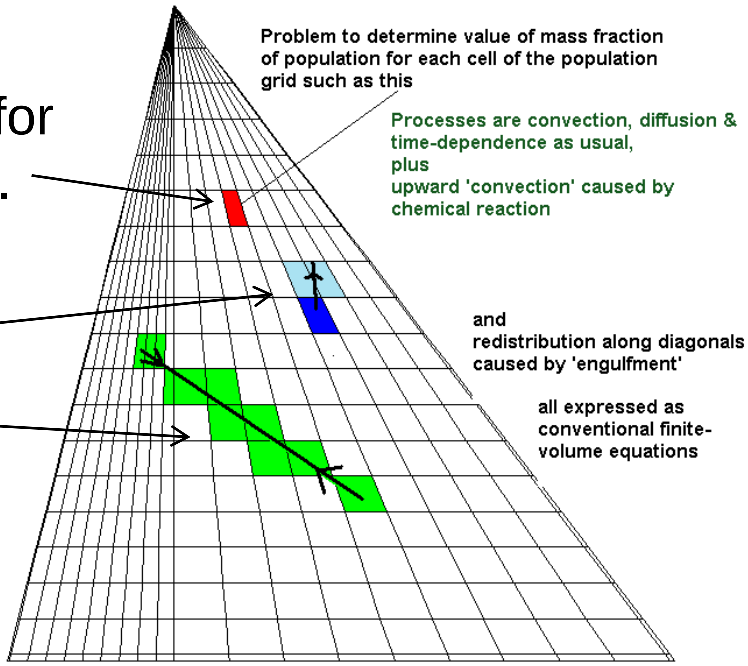
The grid shown on the left is better, using **constant reactedness lines** as the second co-ordinate.

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

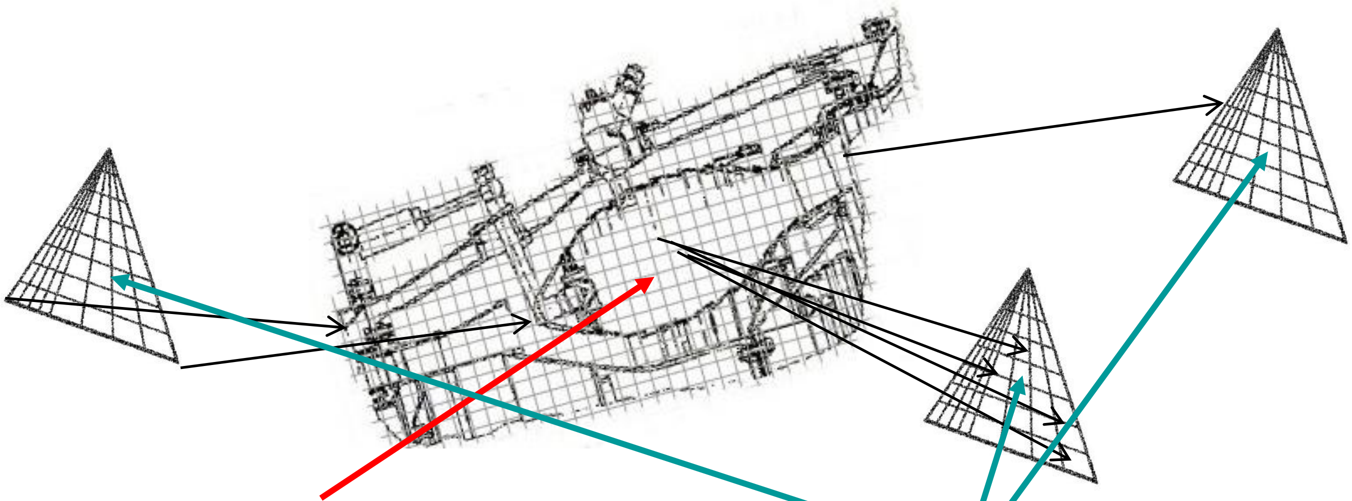
As well as convection and diffusion, these contain terms for reaction

and for engulfment.

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



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



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.

Part 4. Computing population distributions: Final remarks

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Iterative solution presents no problem. ‘Divergence’ never occurs.

Each cell mass fraction is a new dependent variable; so computing time increases in proportion to their number; but it is not immense

Moreover, population-grid fineness *(i.e.* fluid number) need not be the same at all geometrical locations in the combustion chamber.

Further points to note are:

• **Heat loss** to surroundings has been neglected so far, but a single **whole-mixture-enthalpy** equation suffices to allow for it.

• **Differential convection,** *i.e.* differing velocity components, can be handled by **coarse discretisation** for that purpose only**.** Thus the **two-fluid methodology** could distinguish population elements with densities above and below a critical value.

• In summary, the prospects of realistic combustor modelling are good, if EDC, Flamelet, and Pdf-transport can be cleared away.

• And LES too; because the eddies causing engulfment are**’nt** Large!