Preamble: Three **practical reasons** for **computing PTAs and PTBs: Proportions of Time Above and Between**

Marseilles, June 9-11, 2010

8th International ERCOFTAC Symposium on Engineering Turbulence Modelling & Measurement

1. **Death** can be caused by breathing **occasional whiffs** of high-concentration poison-gas, the **time-average** concentration of which may be **not** be **lethal**.

2. It is the occasional **high-velocity gust** which damages the wind turbine, **not** the force of **the time-average wind**.

3. **Explosions** can still occur, even though the mixture as a whole is **too rich** or **too lean** to burn, when **only some** pockets of mixture are **in the flammable range** of air-fuel ratios.

It is **differences from the mean which count !**

PTAs and PTBs; for comparing RANS, LES, 'Multi-Fluid' Models & Experiments by Brian Spalding, CHAM Ltd

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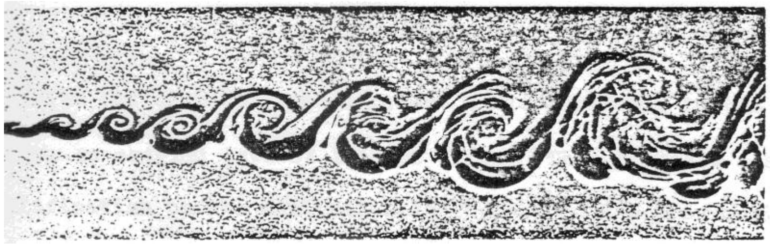
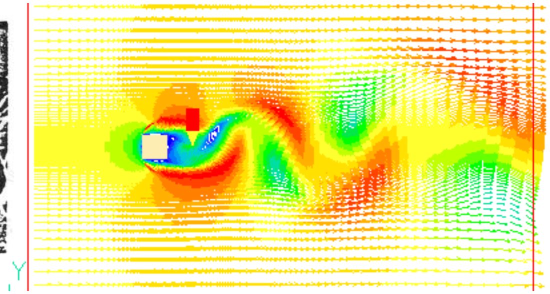
Summary: turbulent flows are transient and fluctuating.

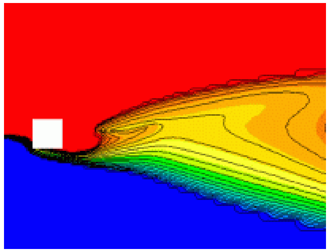




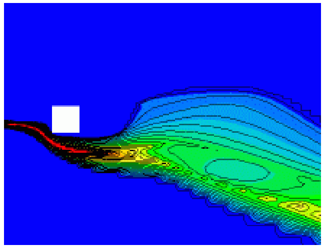
We may need to calculate, say, the **thermal radiation** from them.
Because of the Stefan-Boltzmann T**4 law, this **does not depend** on their **time-average** temperatures.

It depends instead on the **proportions of time in which** the temperature **lies within various intervals** in the range.

So DNS, LES and simpler models should predict the **PTA**s and **PTBs**, *i.e.* **proportions** of time **above ….**



and **between** given values.



Turbulent heat and mass transfer;
What is meant by PTA and PTB

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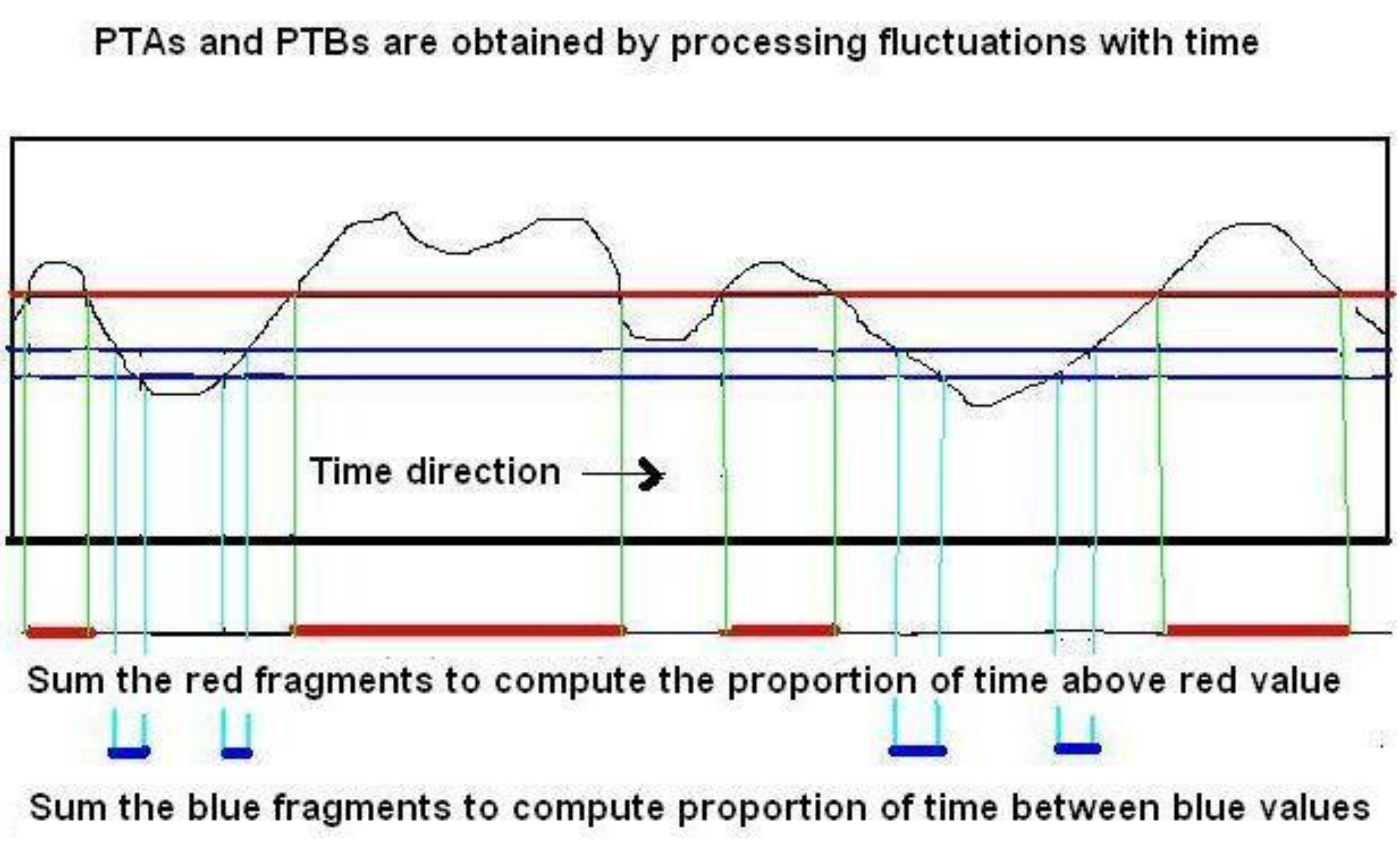


Traditionally, attention is focussed on **surface** aspects of turbulent flows, namely:

- **shear stress** on a wall;
- surface **heat-transfer** coefficient;
- rates of **vaporisation**, **condensation**, **erosion**, *etcetera.*

For many **engineering** purposes, **volumetric** aspects are **equally** important; they influence:

- **visual appearance** (light emission and transmission; obscuration)
- thermal **radiation** and absorption;
- chemical **reaction** including **combustion**, generation of **smoke** and **oxides** of **nitrogen;**
- **noise** emission.

Research publications (*e.g.* of DNS, LES, PANS *etc*) often reflect the **pro-surface bias**; but **volumetric** data are just as easy to present.

Comparisons between results of simulations made by different methods may be **best expressed** in **volumetric** terms.

Therefore both **engineering** and **research** purposes are served by **reporting** the **proportions of time** during which **volumes** are occupied by fluid in defined states; but this is seldom done.

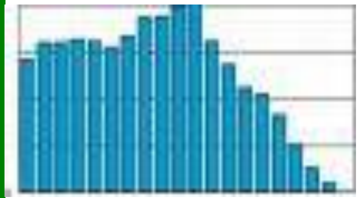
Conventional turbulence **models** (*e.g.* **k-epsilon, Reynolds-stress),** with or without **wall functions,** can **not predict** such proportions **at all;**

but **time-proportion-predicting** models are nevertheless **needed**, for **engineering purposes,** because both DNS and LES are still **far too expensive** for everyday use.

Such models **do exist;** and DNS and LES studies can be used for their **testing** and **calibration.**

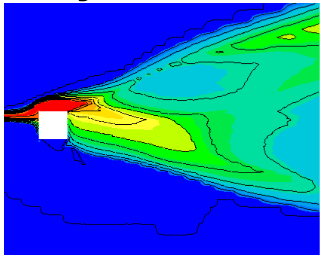
Comparison of fields of **PTA** (= proportion of time **above**) and **PTB** (= proportion of time **between**) provides a convenient means of doing so.

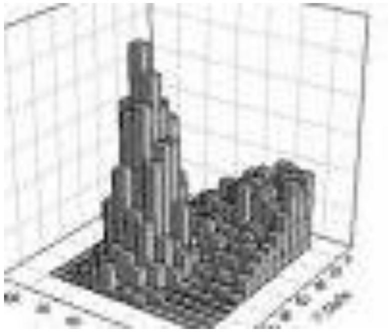
That is the message of the present paper.



PDFs **are** sometimes reported by DNS and LES researchers. They give useful information about **one** location in the flow field and the PTBs of **many states.**

Often however it is **interesting** to know how much fluid, in a **given** state, exists **at all** locations (see right):

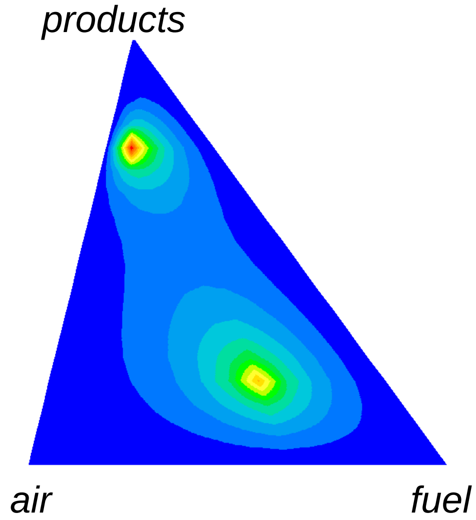




Further t**wo-dimensional** PDFs (left) are needed when two-dimensional fluid-state variations have to be considered. Then PTB **contour diagrams** may be preferable (see right).

The triangular diagram shows the distribution of **combusting-gas** states at a given point in a turbulent flame. The co-ordinates are:

- **Temperature RIse** (vertical) and
- **fuel-air MIXture ratio** (horizontal).



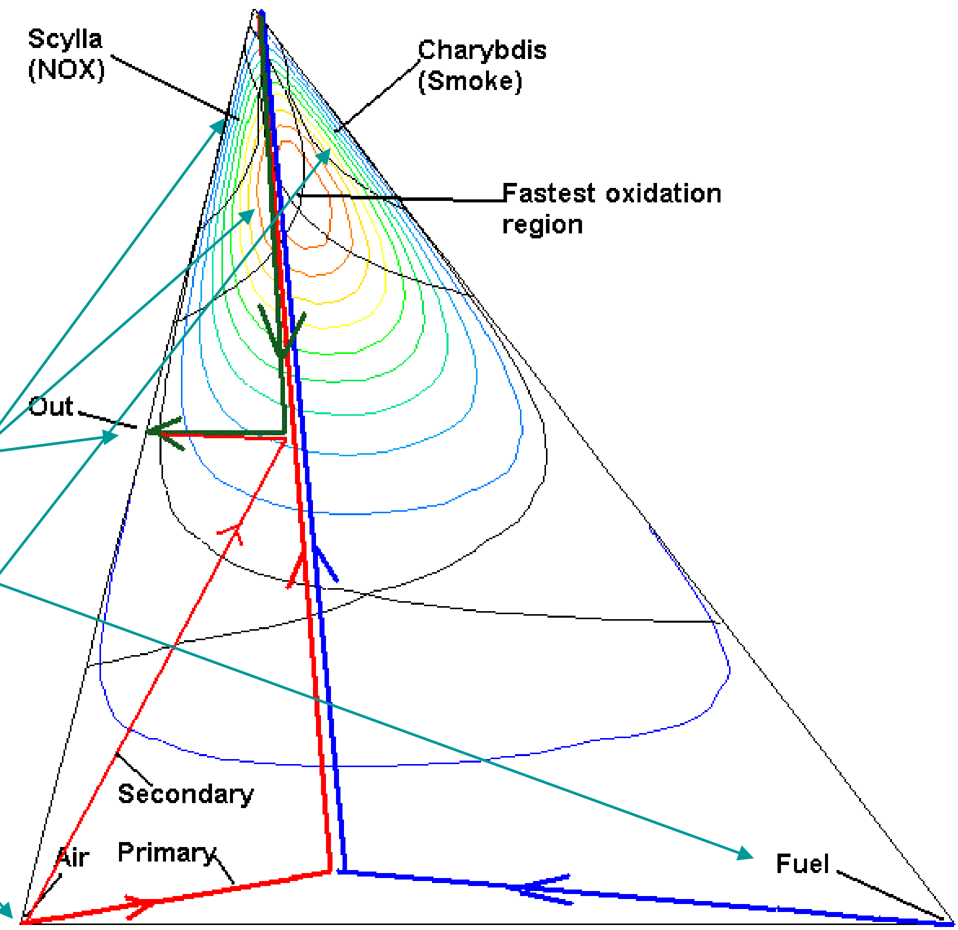
A remark: innovative **display** of results can be as valuable as innovative **research** methods

Example:

The TRIMIX 'map' can **help** gas-turbine-combustor **designers** to 'plot **an optimal route'**

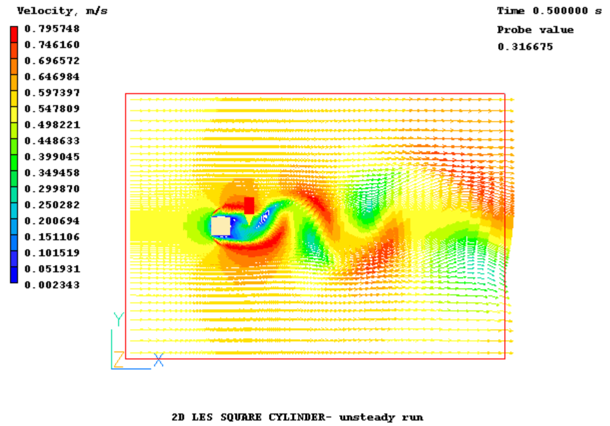
from **reactants** to moderate-temperature out-flow, via the **maximum-reaction-rate** region,

while avoiding the **smoke-generating region** and passing swiftly through that where **oxides of nitrogen** are most copiously produced.

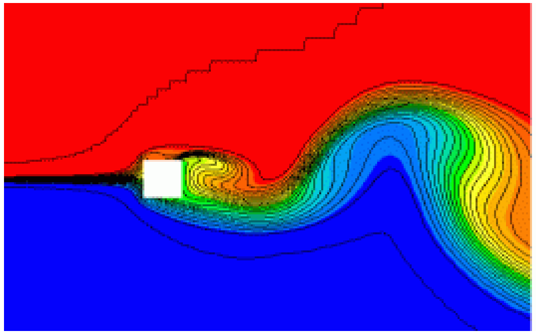


Proportion-of-time calculations; **the current study**

The paper concerns only **non-reacting** flows and the **proportions of time** that **temperature** lies **above** or **between** given limits.



The flow is that behind a square-sectioned obstacle in a **non-uniform** temperature field,

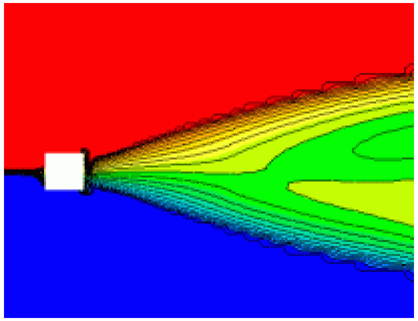


which has perhaps **not been studied** experimentally.

A **two-dimensional LES** simulation was judged sufficient for the present purpose.

Typical instantaneous temperature contours are on the left.

On the right are contours of computed PTA_0.5, *i.e.* proportion of time spent **above** a temperature midway between highest and lowest.



Are they **plausible**? **Who** can decide? And **how**?

Use of PTA fields to answer questions:
Is the number of time steps sufficient?
What is the best value of the Smagorinsky constant?

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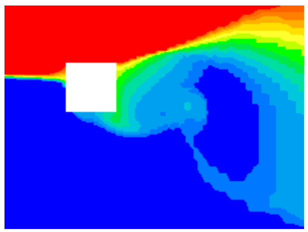
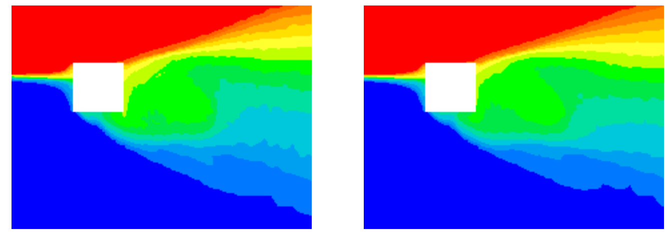
After sufficient time steps LES solutions should become ‘cyclically steady’.

Comparison of PTA=0.9 fields shows how many are needed.



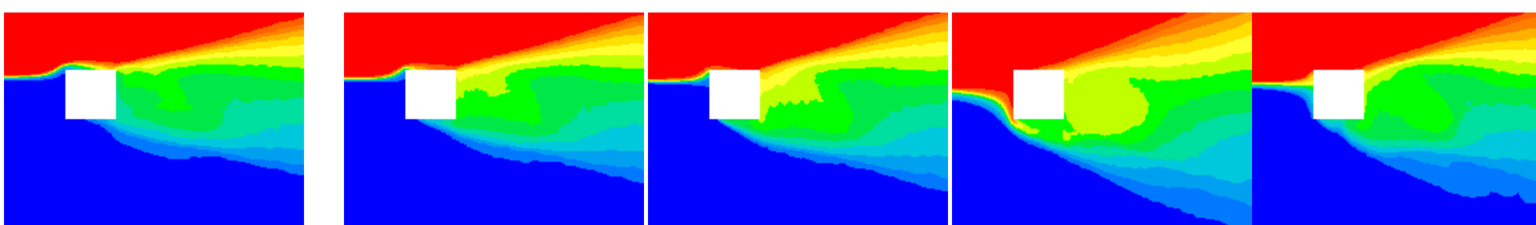
20 time steps is not enough;



but between 100 and 200 time steps, the difference is small.

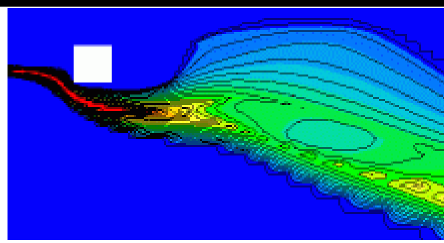
Below are shown **small differences** between PTA=0.9 fields for various values of the **Smagorinsky constant**, namely:

0.2 0.175 0.15 0.05 0.01

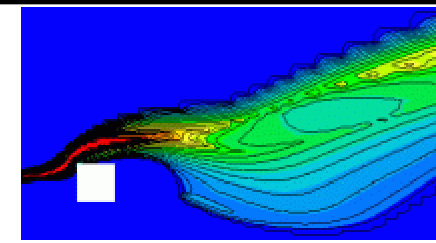


Does it matter at all? Yes: ‘flapping’ almost disappears for Sm const=0.2 .

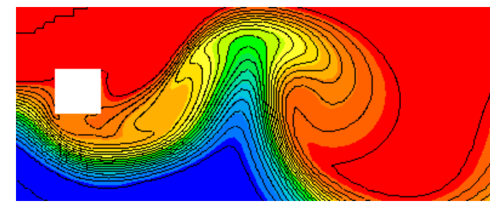
Proportion-of-time calculations; computed PTBs

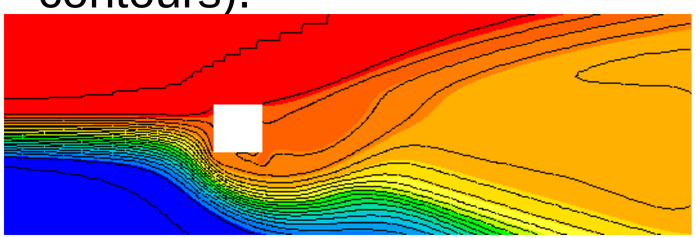


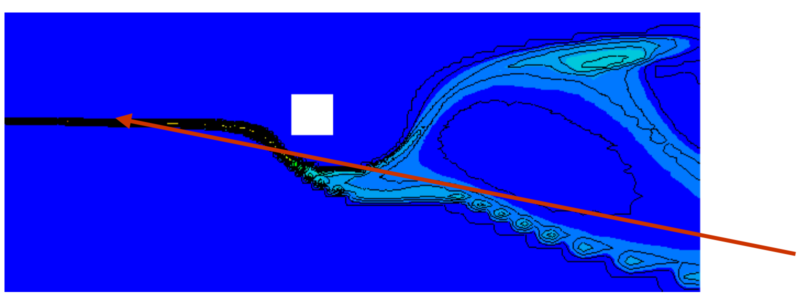
Questions can be asked about PTB_0.-.1 (left) and PTB_.9-1. (right). Are they symmetrical? Should they be?



In the present study, further calculations have been made with the **upper stream-velocity equal to 3 times that of the lower**. The fluctuations continued (see right for instantaneous temperature contours).





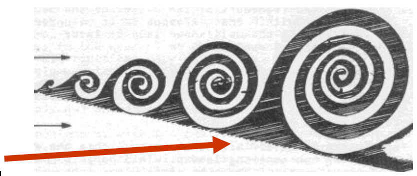


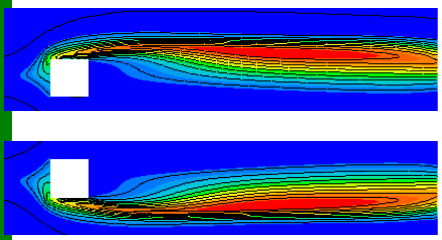
On the left are the **time-average** temperature contours (above) and those of PTB_.5-.5 (below)

They are certainly interesting; but only experiment, or perhaps DNS, can test their correctness.

But note:
the minimal spread of **the upstream mixing laye**r is scarcely plausible.

Multi-Fluid Models of turbulence compute **PTB**s **directly** as **dependent variables** of transport equations with conventional convection and diffusion terms and **additional sources** and **sinks r**epresenting **engulfment**.

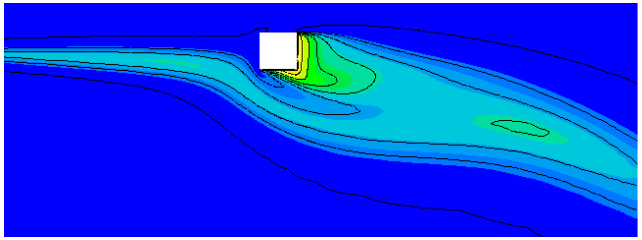




An **MFM** model has been used to predict the **same** two **PTB** distributions as were shown for **LES** on the previous slide, with **only qualitative similarity.**

Quantitative similarity is not to be expected because **k-epsilon** is used for the **hydrodynamics;** it misses the '**flapping**' predicted by LES.

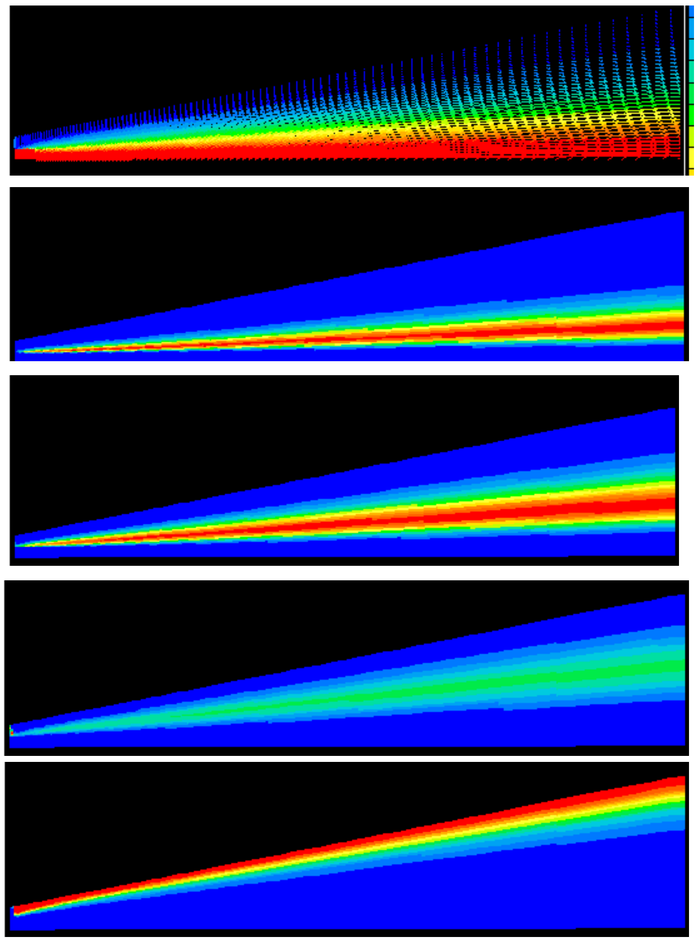
On the right is the **MFM prediction** of the middle-range PTB for the **3:1 velocity ratio.** This **does capture the expected upstream mixing layer**, which **LES did not**.



LES could perhaps have predicted the mixing layer if a much **finer** grid had been used; but the computational **expense** would have been much **greater**.

Proportion-of-time calculations; MFM results from a 1996 mixing-layer study

This finding is not new. Here are results from an earlier MFM study of the **self-similar turbulent mixing layer**, with 40 concentration intervals.



First the velocity **vectors**, lower values above, higher below.

Then contours for the **mass fractions** of fluid in the 10th, 20th, 30th and 40th. **concentration intervals** of upper-stream material.

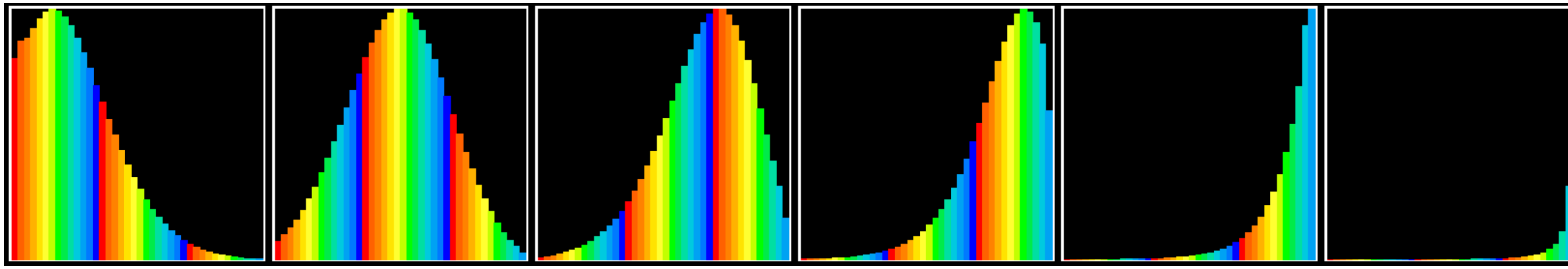
Predictions are in qualitative **agreement** with experimental data.

Quantitative agreement requires (at least) correct choice of the **single adjustable constant.**

The MFM study of the turbulent mixing layer; results expressed as PDFs

The same results can be displayed by way of **probability-density functions**, as shown below. (Note: the colours are for decoration only.)

They are computed for six positions at the downstream boundary successively farther away from the lower (higher-velocity) boundary.



Their shapes differ little if the number of intervals is increased or (moderately) decreased. MFM allows **population-grid refinement.**

Their shapes **do vary** with the value of the **empirical constant**; so comparison with experiment (or DNS) facilitates its choice.

A systematic and comprehensive investigation **remains still to be made**.

Further remarks about the MFM approach to proportion-of time calculation

1. It **exists**, is very **economical,** and gives **plausible** results.

2. The name multi-**fluid** does not imply multi-**phase; 'fluid'** means merely: 'that fraction of the flowing material which lies in a given attribute interval'; A 'fluid' is a **fiction**, like '**cell',** which is its counterpart for **geometric** space.

3. MFMs **differ** from conventional turbulence models in considering a turbulent fluid as a **population,** the elements of which occupy volume for **calculatable proportions of time**, which engineers need to know.

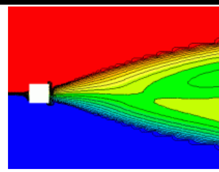
4. They embody **physical hypotheses** regarding (a) exchange of matter between fluids, and (b) relative motion, which require **testing** and **further development**. Constants must be deduced from experiments or DNS.

5. In comparison with LES, DNS, PANS, etc, MFM **explorers are very few**; therefore the **opportunity** for innovative researchers is **wide open.**

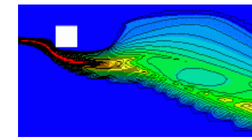
6. The approach is at present the **only practicable** one for engineering use because:

- conventional models (k-epsilon, k-W, *etc*) cannot handle PTA or PTB,
- LES, DNS, PANS, *etc.* are and will long remain **too expensive.**

What the present study may have shown



PTA and **PTB fields** can be used to represent the results of **LES** simulations.

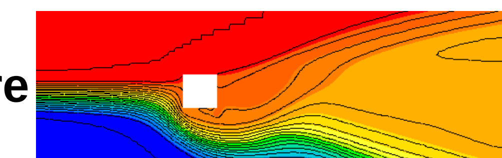


They can and should be used for **comparison**:

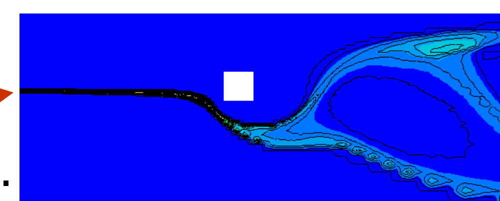
1. **with each other** so as to test effects of grid size, filtering function, cyclical convergence;
2. **with DNS results** to test their conformity with Navier-Stokes equations;
3. **with experiments** to test **realism** more fully than when only **surface-related** phenomena (*e.g.* shear stress) are considered.

They can and should be used, **in principle**, for calibrating MFM models, but have shown that:

• in the **mixing-layer** region **MFM is by far the more plausible**



• that **inadequacies** of the underlying **k-epsilon** model disadvantaged MFM in the **oscillating-wake** region.



• Meanwhile, perhaps no-one can yet say whether these predicted fields are qualitatively right or wrong.

Concluding remarks:
The way forward

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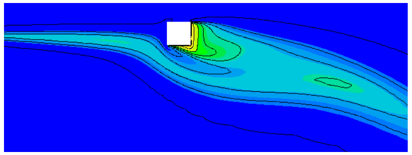
1. It is now widely accepted that, because **both DNS is too expensive** for engineering use**, some combination of RANS & LES** must be employed**.**

2. That is for **hydrodynamics;** but what about **scalar quantities** (*e.g .* temperature,& concentration, which influence **heat transfer, chemical reaction** and **death?**

3. **RANS** (*e.g*. k-epsilon) knows nothing of **PTAs or PTBs;** so **with what** should LES be combined**?**



4. **Answer:** with a **Multi-Fluid Model, which can compute PTAs and PTBs** which LES **cannot resolve.**

5**. How** is this to be done? By **copying** and/or **modifying** the ‘blending’ **techniques already employed** for combining RANS, URANS, PANS, LES, DES, *etcetera.*

6. **When?** Hopefully in time for **ETMM9**.

7. **By whom?** By some members o**f this audience, I hope.**

The end

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and in time for the next large-scale turbulent event:

Thank you for your attention!

Further information about MFM

1. A model-challenging experiment, simulated by a 2-fluid model; slides from a 2008 presentation

2. Slides from a Moscow 2008 presentation with relevance to turbulence in curved ducts

3. Rome 2009: a turbulent-flame presentation

4. A comprehensive early lecture

5. Benjamin Franklin and CFD: a recent presentation

6 Some relevant fortran coding

7 .Marrakech 2008: a presentation with some reference to MFM

Some slides from the Leont'ev birthday conference conference conference; 1

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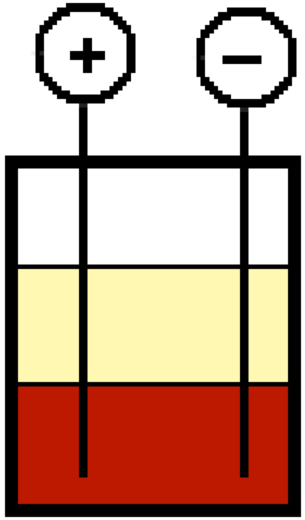
Few CFD packages can simulate the experiment first performed by my student **Lewis Stafford** in 1978, recently repeated by my St Petersburg colleagues **S.Sapozhnikov** and **V.Mityakov**:

- Take a glass-sided vessel.
- Fill the lower half with salty water, coloured by some drops of dye.
- Carefully fill the top half with clear fresh water to create a sharp interface.
- At each end place electrodes, connected to a battery.
- The **temperature** of the better-conducting salty water **rises more rapidly** than that of the fresh.
- So, having earlier been the **heavier fluid**, the salty water becomes the **lighter one**.



Some slides from the Leont’ev birthday conference; 2

- The consequent **Rayleigh-Taylor instability** causes rapid turbulent mixing to occur.
- Within a second, the vessel appears to be filled with coloured fluid.

That process is easy to understand; less easy is what follows if you switch off the electric current as soon as mixing starts and then walk out of the room.
Returning a few minutes later, you will see, perhaps to your amazement, that the fluids **have returned to their original state**: colourless above and coloured below.
They appear to have ‘**un****mixed’**.

How? I will leave you to think about it, giving just one clue:
the molecular diffusivity of salt is much less than the thermal diffusivity of water. Now I shall show a video.

Experiment - video

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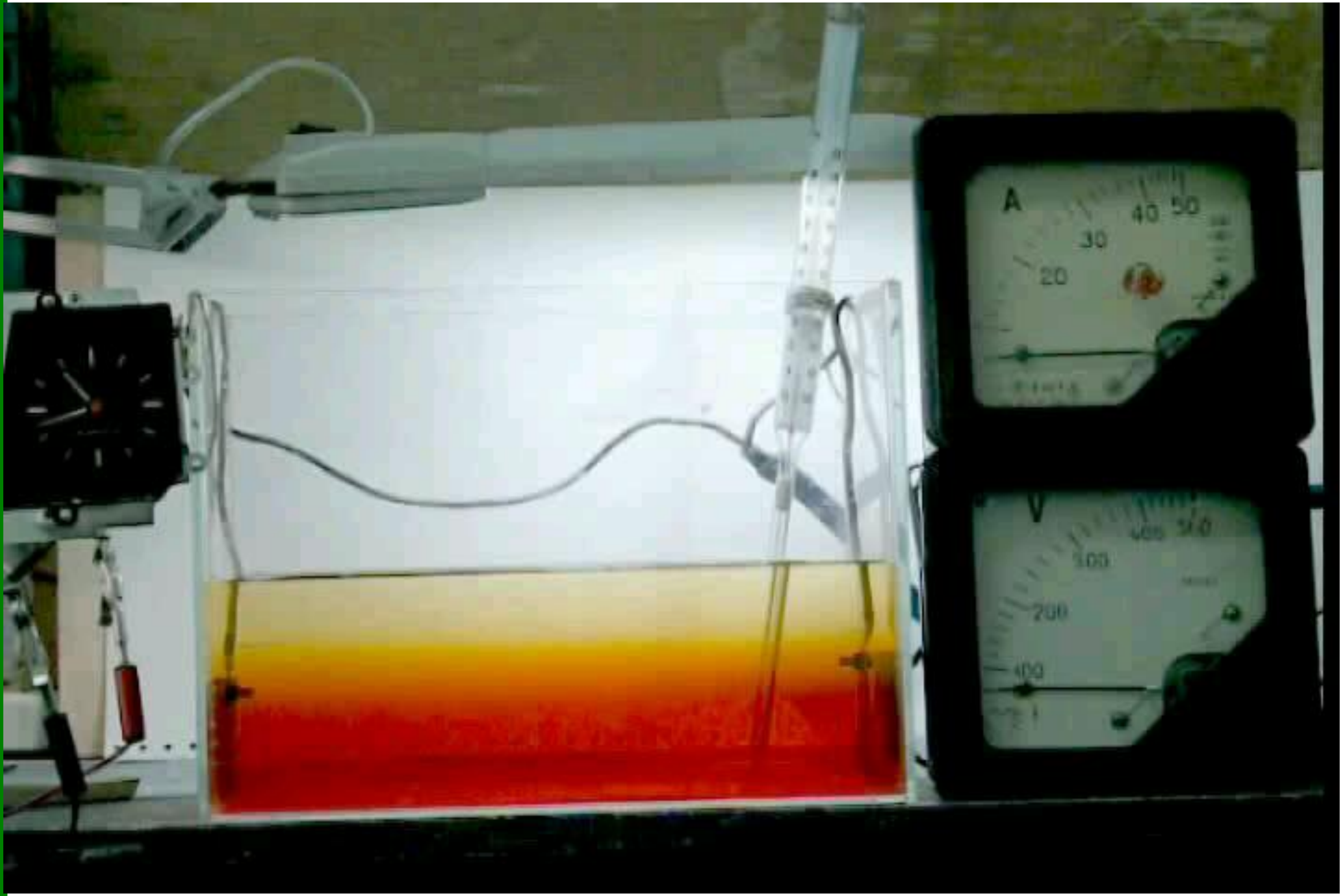
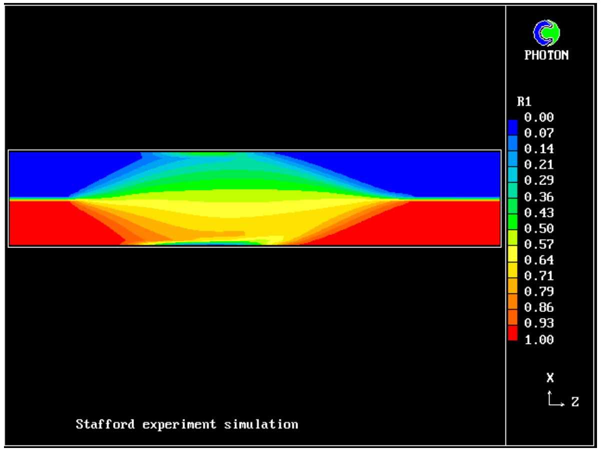


The 'unmixing' process **can** be simulated quantitatively by a **Rayleigh-Taylor turbulence model.** Here is the result of such a simulation:

Contours of the **volume fraction of salty fluid** are displayed.



At the start (on the left), the volume fraction is unity in the bottom half and zero in the top half.

Later (in the middle) fragments of salty fluid rise, and even begin to concentrate at the upper surface.

Later still (on the right), the heating has stopped; so the salty fragments, lose heat to the fresh water and fall down to the bottom again.

The next slide shows more detail.

Some slides from the Leont'ev birthday conference; 4

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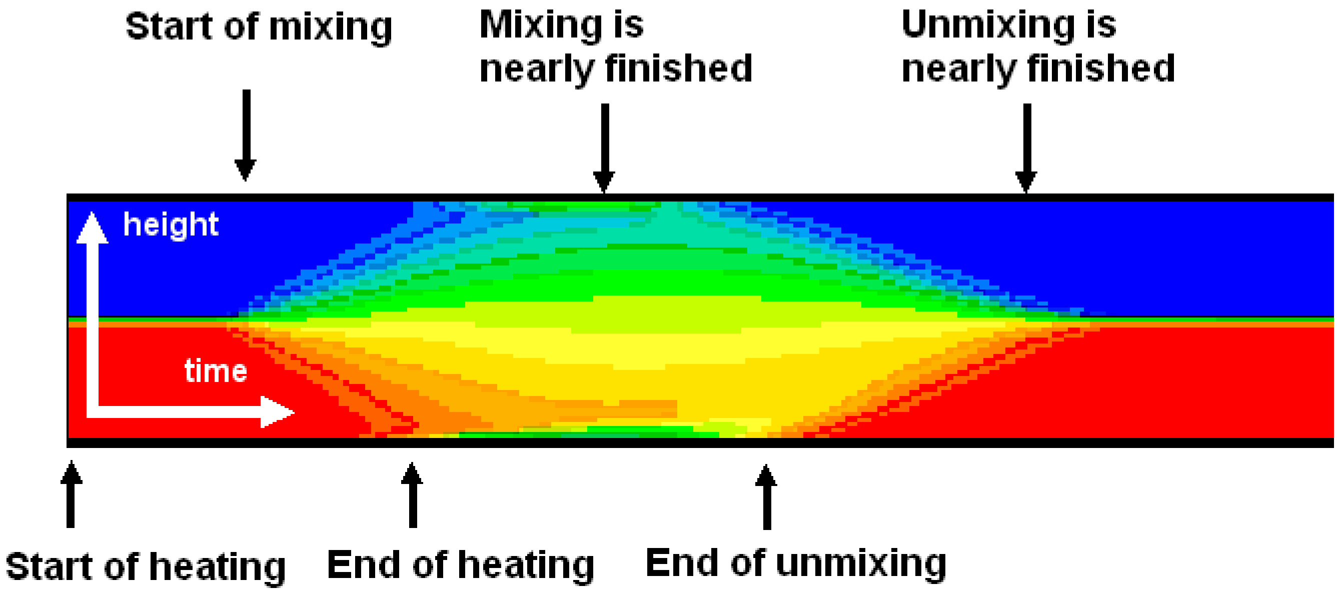
Calculated salt concentration contours; blue = 0.0; red = 1.0



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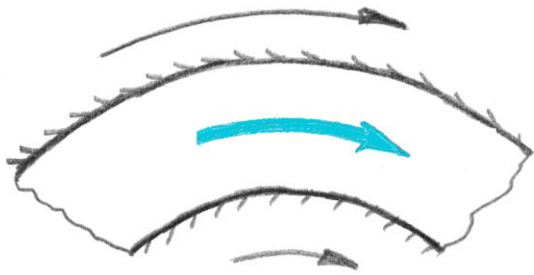
Pure-hydrodynamics opportunities

A '**round-the-bend' idea:** I believe that allowing high-velocity population members to **'sift'** through lower-velocity ones will explain **swirling-flow observations**. Is it not at least worth a try?

4.3 Research opportunities
The ‘round-the-bend’ idea explored. 1

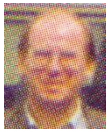
How try?



- Take a **general-purpose CFD code** having **population-dimension** capability.
- Envisage a **turbulent swirling** flow, between cylinders rotating at different speeds.
- Select a **multi-fluid turbulence model,** with **circumferential velocity** as the **population-defining** attribute.
- Choose a high Reynolds Number for which **turbulent-diffusion** and **inter-fluid-collision** processes are of the same order of magnitude**.**
- **Postulate** that radial **‘sifting velocity’** depends on the radial **body forces** being **different for each fluid.** This needs **new thinking**.
- **Vary** this force **systematically,** by changing curvature; then observe the effects on **velocity-population distribution**, shear stress, *etc.*

I have done this, as **anyone** could have done. **A few results** now follow.

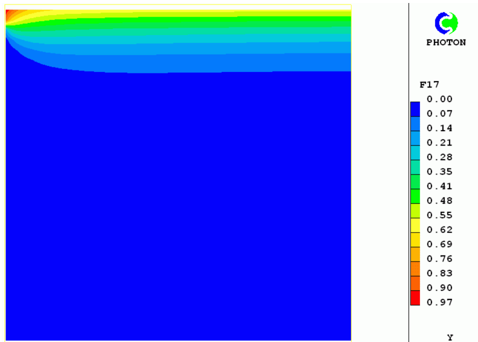
4.3 Research opportunities
The 'round-the-bend' idea explored. 2

1. The general-purpose CFD code which I used was **PHOENICS**.
2. A **steady, rotating, turbulent** flow between two cylinders was set up in a '**switch-on'** manner**.**
3. The **17-fluid model** of Zhubrin  and Pavistkiy  was selected.
4. **Turbulent-diffusion/collision-rate ratios** were chosen, based on **experimental data** for channel flow.
5. **A body force proportional to fluid velocity** was postulated (velocity-**squared** might have been more realistic).
6. A **new** slip-velocity-proportional-to-body-force-difference **hypothesis** was formulated. This hypothesis was **conveyed to PHOENICS** by way of the **In-Form** feature; **no new programming** or executable-building was needed.

The computations, of which the results will be displayed, employed only **standard features** of PHOENICS**.**

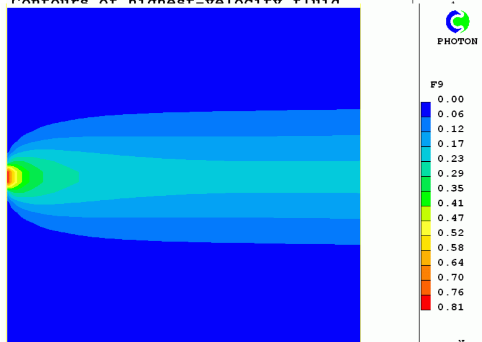
4.3 Research opportunities
The 'round-the-bend' idea explored, 3

Here are results for **zero curvature**, *i.e.* **no** swirl.They are **contours** of **computed mass fractions** of individual population components.
Flow is **from left to right**.
First, the **highest-velocity** fluid, which is clearly concentrated near the upper, higher-velocity wall.



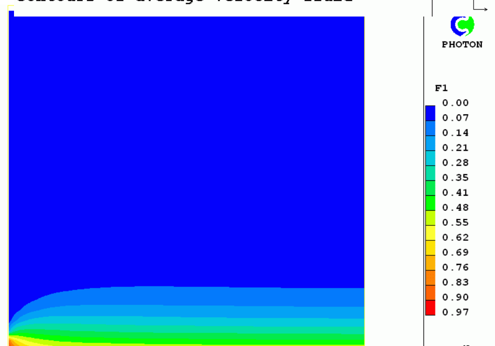
Contours of highest-velocity fluid

Next, contours for the **9th fluid** with velocity equal to the mean wall velocity. They spread as a consequence of turbulent **diffusion opposed by collision.** Downstream cessation of spread implies that the two processes are **in balance**.



Contours of average-velocity fluid

Here are contours of the **lowest-velocity** fluid. Its concentrations are high near the **low-velocity** wall, *ts spread also* **ceases downstream.**



Contours of lowest-velocity fluid

Diagrams for **all 17 fluids** have been computed; but to display them all would be tedious.

4.3 Research opportunities
The ‘round-the-bend idea explored, 4

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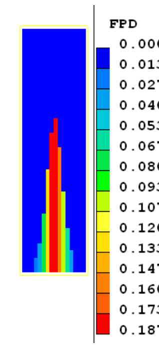
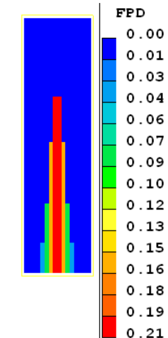
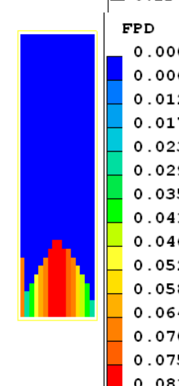
The **fluid-population distributions** (**FPDs**) have also been computed. Here is that for the **central plane**, when the duct is **not curved**. **Fluid-9** has the highest mass fraction, *viz* 0.187**.** **Results** for **curved ducts** will now be shown**.**



Here is the corresponding FPD for **radius increasing with** average velocity; the distribution becomes **narrower .**
The **fluid-9 mass fraction has risen** to 0.21.
Faster fluids **sift** towards **the faster-moving outer wall.**



Now the **direction of curvature is changed**. Faster-moving fluids now **sift away from** the faster-moving, **now inner** wall.
The shape of the FPD **broadens** dramatically. **Fluid-9 mass fraction has fallen** to 0.81, and the **shear stress increases**.



These results explain why flows near **convex** and concave walls are so **different**. Only **population models** can begin to simulate **swirling- flow behaviour.**
They should be **vigorously developed** and **used.**.