Population models of turbulent heat and mass transfer

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Rome, Italy
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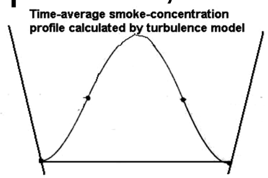
6th International Symposium on Turbulence, Heat and Mass Transfer

Summary

Conventional turbulence models handle only **macro-**mixing**.**

They calculate the **time-mean** concentrations in plumes, arriving at skimpy, reality-missing results *e.g.* for the '**profile**' across the plume like this->

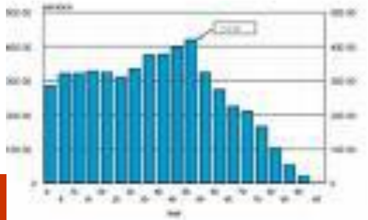


Population models of turbulence handle **micro-**mixing **in addition.**

They are **needed** for **realistic** prediction of **non-linear** processes such as:
* thermal **radiation**, * chemical **reaction**, * **biological** response,
* **fluid-structure** interaction, * **condensation** and evaporation, * ***etcetera.***

Population models of turbulence predict **probability-density functions.**

They **discretize** these **pdf**s. Then they treat the histogram ordinates as dependent variables of individual **conservation equations** .



'They also allow **population-grid refinement**'.

Population models of turbulent heat and mass transfer; how turbulent mixing proceeds

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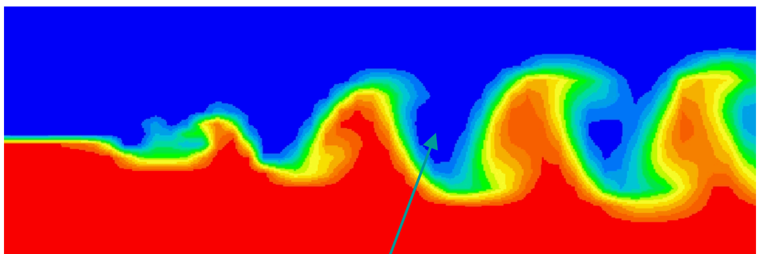
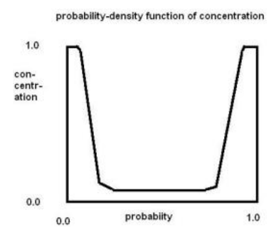
Boussinesq's enlarged-viscosity concept predicts **macro-mixing** well, but not **micro-mixing.** It is **eddy roll-up**, enlarging interface **areas** and concentration **gradients,** which allows **laminar diffusion** to do its work.

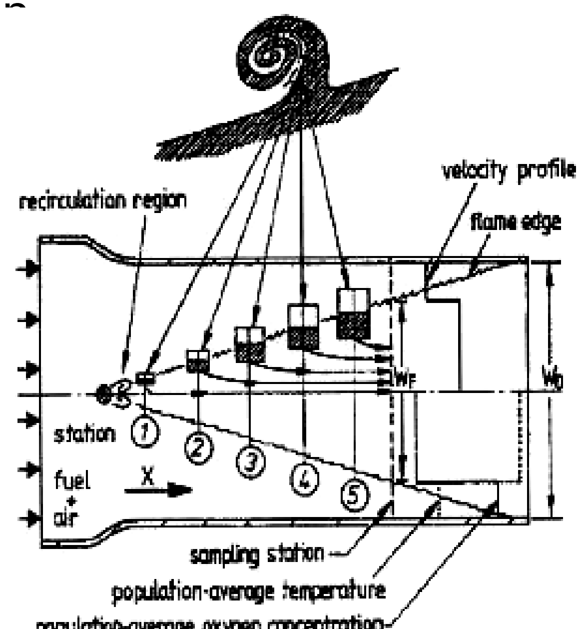


On the left is Urban Svenson's 1998 numerical simulation of the **Kelvin-Hemholtz** instability which causes eddy roll-up.

The **probability-density function** for this **location** will look like **this**:

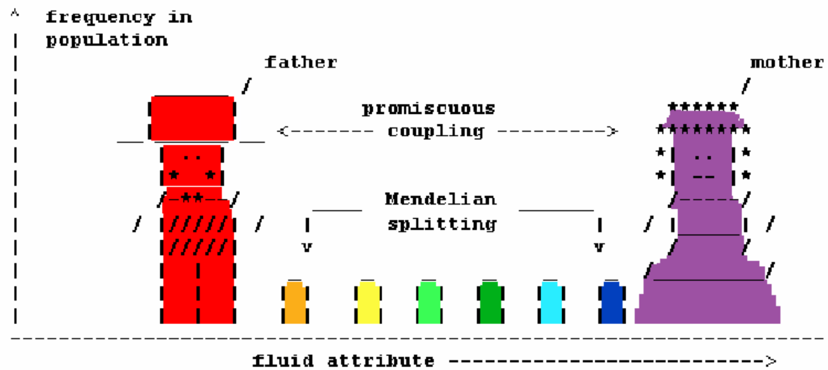


On the right is a sketch of the 1970's **'ESCIMO'** concept of how '**Engulfment**' and '**Stretching**' **increase gradients** of temperature and concentration and so facilitate chemical reaction (Noseir, 1980).



• In what follows, **transient engulfment** and **stretching** processes are postulated as occurring **continually and throughout** the turbulent fluid.

• They can be likened to '**brief encounters'** between unlike parents, leading to offspring of **intermediate complexion**, as illustrated here:



• In the absence of other guidance, the **rate of offspring production** is taken as proportional to the **parent-concentration product**, times:

*the square root of the sum of products of **velocity gradients**.*

• This square root, multiplied by the effective viscosity, represents the

***generation rate** of turbulent kinetic energy,*

linking conveniently with hydrodynamic turbulence models *e.g*. **k-epsilon.**

• The **pdf**'s (now also called ***population distribution*** **functions**) of **complexion** are then computed *via* simple **mass balances**.

Population models of turbulent heat and mass transfer; some history

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- The use of mass-balance (*I.e.* 'pdf-transport') equations for computing population distributions was proposed by **Dopazo** in 1975.

- Numerical solutions were first provided in 1981 by **Pope**, who (wisely?) chose the **Monte-Carlo** method for doing so.

- Computations by **Fueyo** (2008) for hydrocarbon combustion, shown here, were also obtained by the Monte-Carlo method.

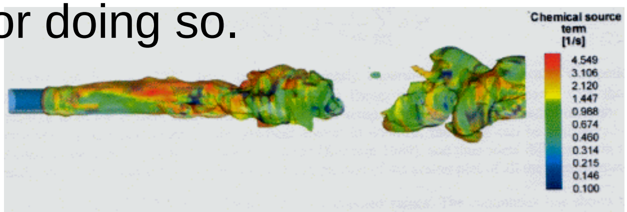
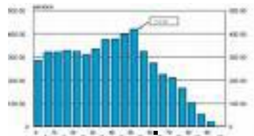
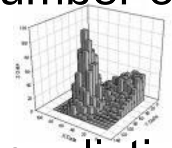


Figure 7. Instantaneous flame structure. Top: isocontours of OH in LES calculation; middle: isocontours of reaction rate in LEM calculation; bottom: isosurface of stoichiometric mixture

- In 1996, independently and as a generalisation of the 1971 '**eddy-break-up**' concept, I created the **'multi-fluid model'**.
This **discretized the pdf**, treating the histogram **ordinates** as the dependent variables of a sufficient number of differential equations.

- Both **1D**  and **2D**  histograms were used; and attention was given to **how many** distinct 'fluids' (*I.e.* histogram ordinates) were required for for accuracy.

This **population-grid-refinement** possibility, not available in the Monte Carlo method, is an advantage of the discretized approach.

Population models of turbulent
heat and mass transfer;
questions which **research** could answer**.**

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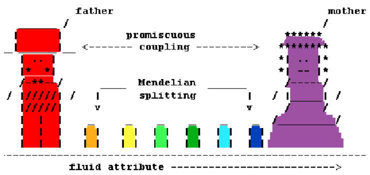
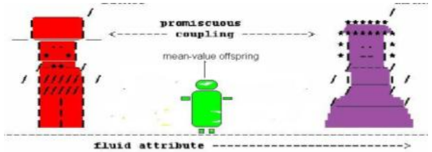
1. The **'offspring-production-rate' equation** contains a proportionality constant (**CONMIX** below) which must be obtained from **experiment**.

- What is its **value**?
- **Is it** indeed a constant?
- If not, does it depend on **Reynolds Number**? on **energy-dissipation/production-rate ratio**? on **something else?**

2. Are 'complexions' of the offspring **distributed** In uniform **'Mendelian'** fashion shown on the right)?





Or is there just one offspring complexion, as shown on the left?

3. Pdf's of temperature are **easy to measure**; and their **shapes** depend on the assumptions made for CONMIX and offspring distributions. Therefore the research questions can be answered, by **comparing** with experimental contour and pdf shapes and sizes (see next slides).

4. Unfortunately few researchers practise **both** experimental and numerical studies. How to change **that** is the **most pressing research challenge.**

Results will be presented for the much-studied steady **axi-symmetrical uniform-density turbulent jet.**

The **macro-mixing** part of the model is **conventional** in that:
• the **k-epsilon model** is employed for the calculation of the **effective viscosity;** and
• a constant **effective Prandtl number** characterises the turbulent diffusion of each of the hypothetically distinct fluids.

The **micro-mixing** part of the model is **unconventional**, in that:
• each equation has a **source term** which expresses its rate of creation by the evening out of the steep concentration gradients within the engulfed eddy; and
• it has a corresponding **sink term** expressing its contributions, with partnering ‘parents’, to new engulfments.

If this mingling of disparate elements is adjudged inconsistent, so be it. Consistency is not always a virtue.

Population models of turbulence; fluid-concentration contours for a **steady axi-symmetrical jet** with CONMIX=100

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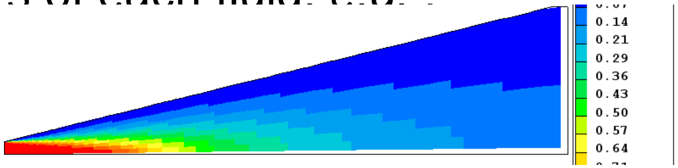
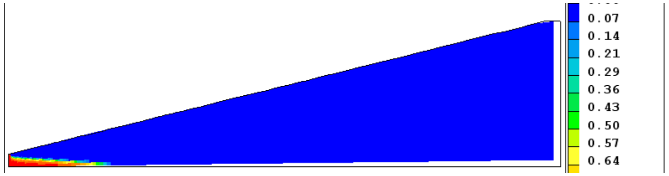
Numerical simulation with a **20-fluid model** and a 20*100 spatial grid leads to concentration contours of each fluid, *e.g.* :

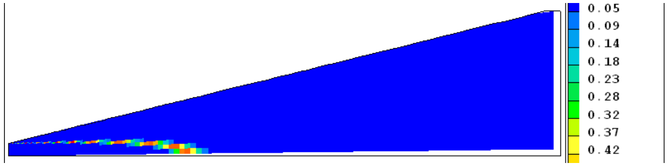
1. Sum of all 20 fluids, *I.e.* the conventional mixture fraction



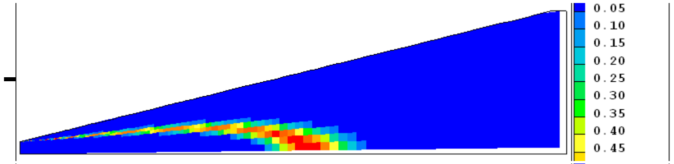
2. Fluid 1, of highest injected-substance concentration



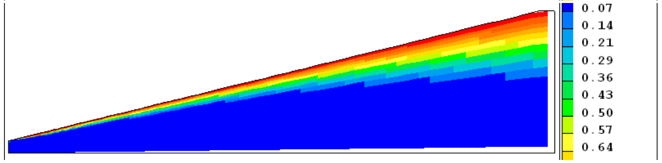
3. Fluid 10, of smaller injected-substance concentration



4. Fluid 15, of still smaller injected-substance concentration



5. Fluid 20, of smallest injected-substance concentration

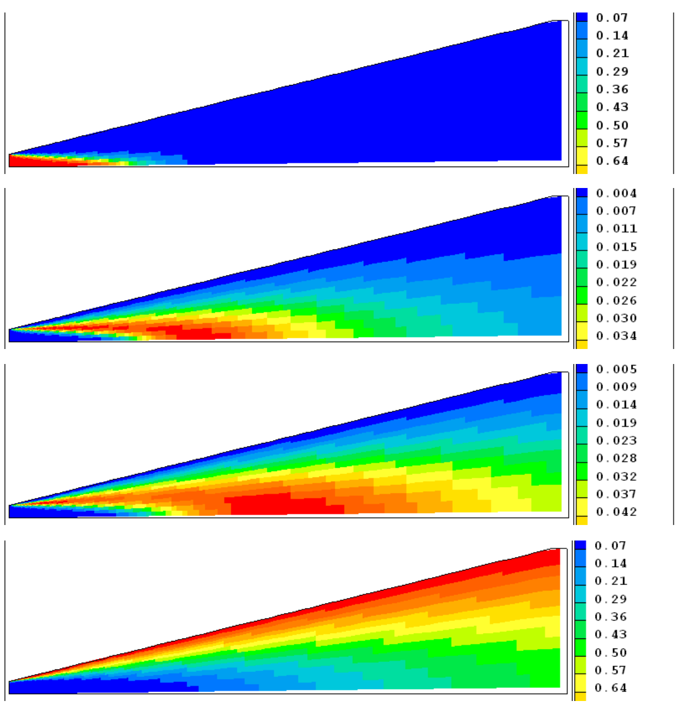


Note that 20 additional differential equations had to be solved!

Population models of turbulence; fluid-concentration contours for the jet, with **CONMIX=1 and 100 compared**

With CONMIX=**1** (on the left) the contours are **much broader** than with CONMIX=**100** (on the right, as just seen). Which are the **more realistic**?

The '**true**' value of CONMIX can be established by **comparison** of experimentally-measure **pdf's** with calculated ones (see next slide).

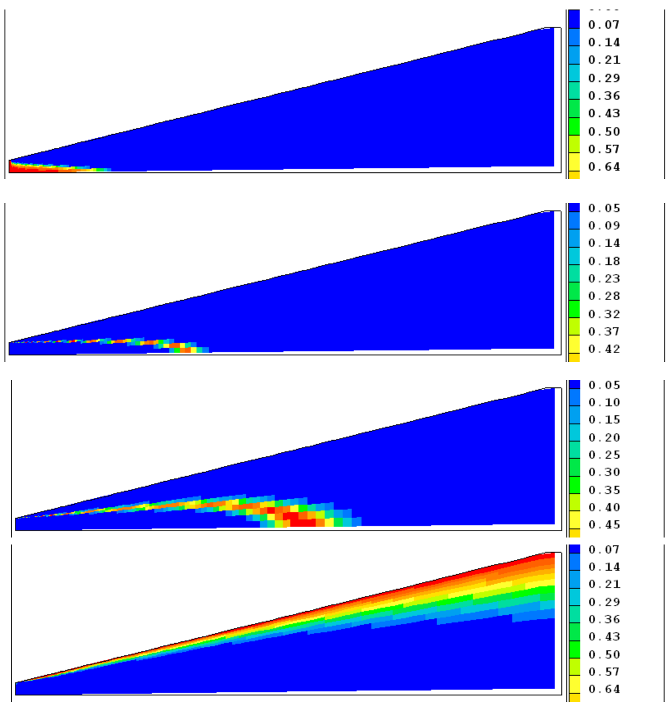


Fluid number:
1

10

15

20



Population models of turbulence; pdf's at two points on the jet axis, for CONMIX=1, 10 and 100

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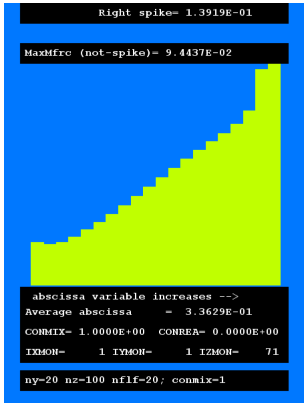
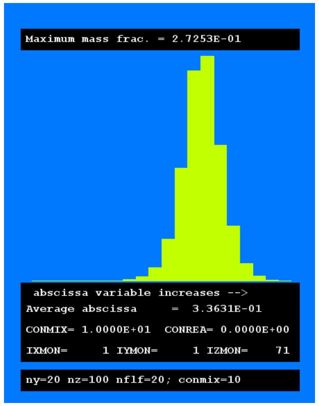
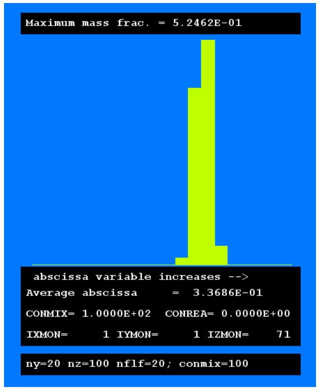
Computed pdf's for CONMIX =

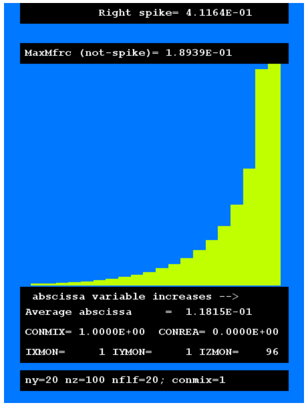
1.0 10.0 and 100.0

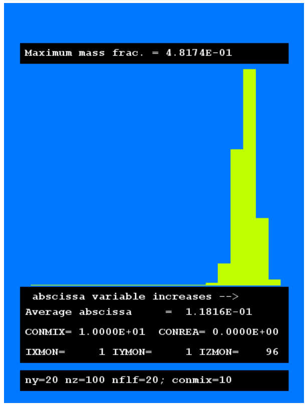


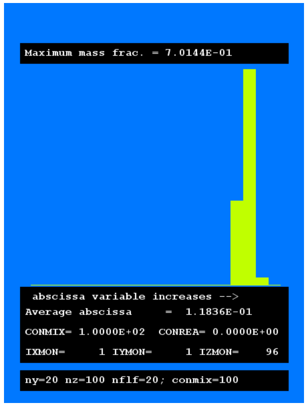




Axial distance nozzle diameter = 10







Axial distance nozzle diameter = 18

Such large shape differences should make it easy to determine CONMIX

Population models of turbulent heat and mass transfer; **population-grid-refinement** effects

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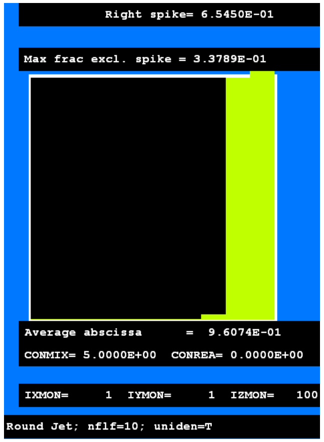
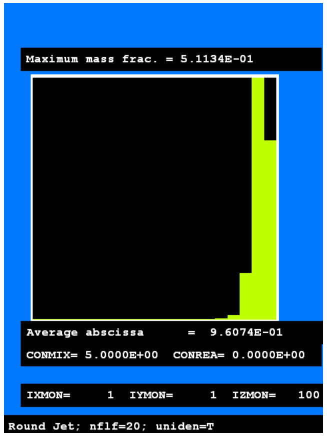
Perhaps the 20-fluid model gives **insufficient resolution** of the pdf; therefore it is instructive to **vary the 'population-grid' fineness**, as shown below, for CONMIX= 5, for a point on the axis far from the nozzle.

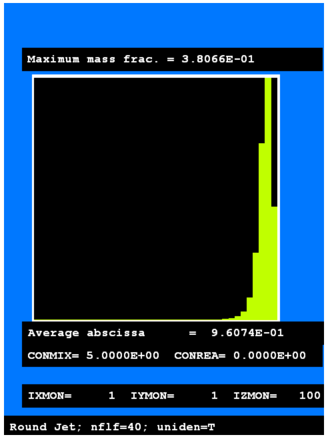
Number of fluids = 10



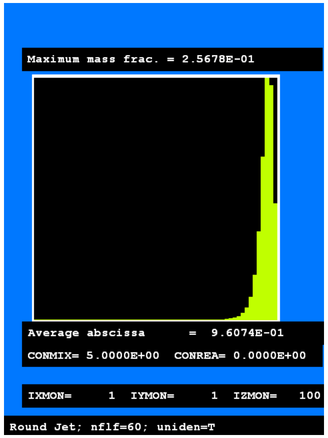
= 20



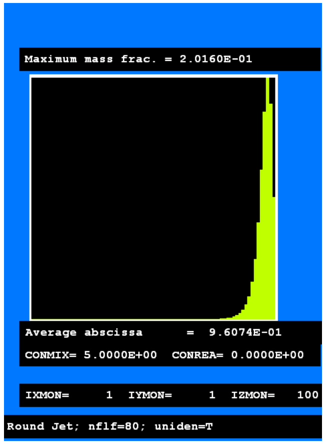
= 40



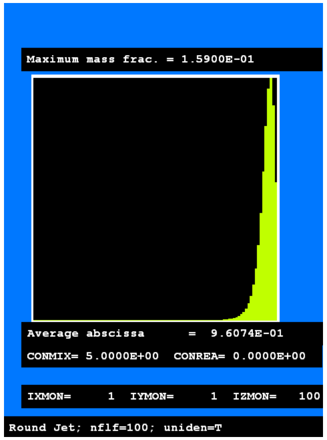
Number of fluids = 60



= 80



= 100



comments on the foregoing results

1. Increasing the number of fluids does give the **expected smoothing** of the pdf shape; and it of course increases the computer time also.

2. Computer times are however very **small** (less than 1 PC minute).

3. The program was PHOENICS, which has a **built-in** (but user-adjustable) **multi-fluid model** and a library of input files.

4. What is now needed is that **experimental researchers** should **use it**, or some equivalent software.

5. It is also desirable that **Direct Numerical Simulation** (DNS) practitioners should **post-process their results in terms of pdf's** and of the quantitative conditions which influence them.

6. Aiding turbulence modellers in this way may be regarded as **the main useful result** which can emerge from DNS studies, until computing power increases greatly.

7. But the modellers need to **abandon conventional Kolmogorov-type** models and **"think pdf".**

1. Death can be caused by breathing **occasional whiffs** of high-concentration poison-gas, the **time-average** concentration of which may be **non-lethal**.

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

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

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

Four **common misconceptions** have been challenged, namely:

1. That turbulence models **must be** of **Kolmogorov** type, concerned only with **mixture-average** quantities, *e.g.* k, epsilon, RMS fluctuations, *etc.,* perhaps with **presumed pdf shapes.**

In fact, the pdfs of any fluid attribute (or pair of attributes) can be computed directly, with few and **testable** assumptions.

2. That Monte-Carlo methods **must be** used for computing pdfs.

In fact, **discretization** is simpler (to understand and to program), and more informative; moreover it allows population-grid refinement studies.

3. That CFD has **at most 4** dimensions (3 of space and 1 of time).

In fact, it must become **multi-dimensional** if the **population-related** aspects of fluids are to be simulated

4. That turbulence modelling is a **unique activity**, unlike any other.

In fact, it is just one branch of **population modelling,** of which other branches concern: particle-size variation, bacterial growth and decay, animal-species interaction, *etcetera.*

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Thank you for your attention!

The End