Turbulence models for CFD in the 21st century

by

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Abstract

The two approaches to turbulence modelling

Both Osborne Reynolds (1884) and Ludwig Prandtl (1925) regarded turbulence as an expression of the near-random **intermingling of sizeable fragments** of unlike fluid, which, during a succession of brief encounters, tended to equilibrium.

However, their concept **found no place** in the family of turbulence models springing from **Kolmogorov's** (1942) proposal to attend only to **statistical measures** of the turbulent motion, such as energy and frequency.

The intermingling-fragments idea was nevertheless preserved in the models of Spalding (1971) and Magnussen (1976) ("**eddy-break-up**" and "**eddy-dissipation**", respectively) which are still used for combustion simulation.

It also featured in Spalding's (1987) **"two-fluid" model** of turbulence; and it is essential to the **"multi-fluid" models** of turbulence (Spalding, 1996) which are the subject of the present lecture.

Why the Kolmogorov approach has been popular until now

Limitations of computing power, and the seeming simplicity of the associated (1877) effective-viscosity concept of Boussinesq (1877), favoured adoption of the Kolmogorov rather than the Reynolds-Prandtl approach; and this road has now become so well-trodden that most CFD practitioners suppose, wrongly, that it is the **only** one which is open.

This would not matter if Kolmogorov-type models, for example **k-epsilon** (Harlow and Nakayama (1968)), allowed computation of the "**probability density functions**" needed for the simulation of non-linear processes such as radiation and chemical reaction; or if they could comprehend such real processes as "**un-mixing**"; but they do not.

Why the Reynolds-Prandtl approach is likely to be favoured from now on

"Intermingling-fragments" models of the kind conceived by Reynolds and Prandtl, **do** however permit these things; and the computing power needed for using them is easily available nowadays.

The lecture will explain how such "multi-fluid models" may be:

a. formulated
b. calibrated
c. utilised for simulating engineering processes and equipment,
d. subjected to numerical-accuracy tests, and
e. further developed.

Similarities to, and differences from, the "pdf-transport" models of Dopazo and O'Brien (1974), and of Pope (1982), will be pointed out.

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1. Alternative concepts of turbulence

- **Boussinesq** (1877) postulated that a turbulent fluid could be treated like a laminar one with **enlarged viscosity**.
  - This postulate was adopted by **Kolmogorov** (1942) when he proposed **differential equations for statistical properties** of the turbulent motion, from which the local values of the enlarged viscosity could be computed.
  - Nearly all currently-used models follow the Boussinesq-Kolmogorov line.

- The best-known is that of Harlow and Nakayama (1968), namely the **k-epsilon** model.

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- **Reynolds** (1884) postulated that a turbulent fluid could be better understood as a near-random mixture of **intermingling fragments**. Thus:
  - Reynolds envisaged **hot fast-moving fragments** flung from a fluid stream as making **brief contact with a cold wall**, whereafter they are plucked back into the stream as **lower-moving, cooler fragments** .
  - This concept was the basis of the **Reynolds analogy** between friction and heat transfer.

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  - **Prandtl** (1925) envisaged similar **to-and-fro movements**, with exchanges of heat and momentum between fragments as they passed or collided, also **throughout the volume of the stream.**
  - This was an essential ingredient of his **mixing-length hypothesis.**

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- Enlarged-viscosity models become popular in the 1970 when the first computers, and the earliest CFD programs, allowed the Komogorov-type differential equations to be solved.

- However, the intermingling-fluid concept survived in the **combustion community** (Spalding,1971; Magnussen and Hjertager, 1976), because flames can be understood **only** as **intermingling fragments** of:
  - hot, fully-burned gases,
  - cold, un-burned gases, and
  - gases of intermediate temperature and composition.

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- It will be argued below that because:

  a. the limitations of the Kolmogorov (statistical-properties) approach have proved rather severe,

  b. the **multi-phase-flow community** has shown that the intermingling-fragments equations **are now also easy to solve** (eg Spalding, 1987),

  it is time to give switch attention to models based on the Reynolds-Prandtl concept.

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2. An enlarged-viscosity model: LVEL

- **Enlarged-viscosity models do still have a part to play,** especially when friction and heat transfer in non-reacting fluids are of major concern. Particularly useful is the so-called LVEL model (Spalding, 1994), which is often to be preferred when solids of complex shapes are immersed in fluids.

- Such problems arise in electronics-cooling problems, where it is often desired. in addition, to **compute simultaneously the stresses and strains within the solids**.

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- The LVEL model computes the value of the enlarged viscosity at any point from:
  - The fluid velocity at the point,
  - The distance of the point from the wall,
  - The "Universal Law of the Wall".

- Space does not suffice here to describe the method; but an example will be shown, during the oral presentation.

Example 1: An SFT (solid-fluid-thermal) problem

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- Points to note are that LVEL:
    - embodies an economical method of computing the **distance from the wall**;
    - predicts reasonable values of the enlarged viscosity for both **low** and **high** Reynolds Numbers;
    - is compatible with the simultaneous computation of the **stresses and strains** within the solid.

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- Therefore, although simple and unpretentious, the author includes LVEL in his list of turbulence models for the 21st Century.

- It does however require further development, for example by allowing the length scale to be diminished by local velocity gradients as well as by distance from the wall [**Researchers seeking opportunities: please note!**].

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3. Where enlarged-viscosity models fail

- There are however many practically-important turbulent-flow processes which defy simulation by any Boussinesq-Kolmogorov-type (ie "thick-soup") model. One of these will now be described.

- A salt-water layer, lying below fresh water, is heated for a short time by an electric current.

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 ___________        ___________        ___________
|           |      |* * ** * * |      |           |
|   fresh   |      | * *  * * *|      |           |
|           |      |* * ** *  *|      |           |
|***********|      | * *  * ** |      |***********|
|** salty **|      |* * ** * * |      |***********|
|***********|      | * *  * * *|      |***********|
 -----------        -----------        -----------
   start               later           later still
  un-mixed            mixed ?        un-mixed again !
```

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- Mixing appears to take place soon after **heating equalises the densities**.
- But it is **macro- not micro-**mixing; and, because the Prandtl and Schmidt numbers differ,the **"intermingling fragments"** transfer heat by conduction more rapidly than they exchange salt by way of diffusion.
- Therefore **"unmixing"** takes place.

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- This process can be correctly simulated by even the first of the intermingling-fluids models to be expressed by way of diffferential equations (Spalding, 1987), as will be demonstrated during the oral presentation.

  Example 2: Two-fluid simulation of the mixing/unmixing experiment

  Only those CFD models which incorporate the Reynolds, intermingling-fragments, concept can simulate such phenomena.

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- Related phenomena which require IFMs for their simulation include:-
  - the reduction in the shear stress in a turbulent boundary layer when it passes over a convexly curved wall;
  - the "bumpiness" of low-altitude airplane rides over sun-heated terrain;
  - the mixing of blade wakes with between-blade gases in turbo-machines
  - the Ranque-Hilsch effect;
  - almost all processes involving chemical reaction in turbulent gases.

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4. Why intermingling-fragment models (IFMs) can simulate a wider range of phenomena than EVMs

- Interminging-fragments models, or "multi-fluid models" (MFMs) to call them by a more common name, **compute the "PDFs"**.

  This acronym serves equally well for:-
  - the **"probability-density functions"**, which feature in mathematical representations of the fluctuations with time of instantaneous values of velocity, temperature or other practically-interesting properties; or
  - the **"population-distribution frequencies"**, which is the term used in the MFM literature.

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- PDFs of the second kind can be regarded as **discretised** versions of PDFs of the first kind.

- They take the form of **histograms**, whereby:

  - the **ordinate** represents the proportion of the population

  - lying within the corresponding **abscissa** interval;

  - and the abscissa stands for the **population-distinguishing attribute** in question, for example:
    - temperature
    - fuel concentration
    - vertical velocity
    - etc

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```
^      __    a one-dimensional "PDF""
|     |ÝÝ|                        __
|     |ÝÝ|                       |ÝÝ|
|     |ÝÝ|          |ÝÝ|__       |ÝÝ|
|     |ÝÝ|        __|ÝÝÝÝÝ|      |ÝÝ|
|     |ÝÝ|__     |ÝÝÝÝÝÝÝÝ|__    |ÝÝ|
|     |ÝÝ|ÝÝ|  __|ÝÝÝÝÝÝÝÝÝÝÝ|__ |ÝÝ|
|   __|ÝÝ|ÝÝÝ__|ÝÝÝÝÝÝÝÝÝÝÝÝÝÝÝÝÝ|__|ÝÝ|__
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  --- population-defining attribute ---->
    for example temperature or concentration
                        ^
population-mean value _|
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- **Knowledge of PDFs is essential** whenever important phenomena depend in a complex fashion on the population-distinguishing attribute.
- For example, the **thermal radiation** or the rate of **chemical reaction** will be quite different for:

    1. a gas mixture having the PDF just shown, and
    2. a gas which is completely mixed and so possesses the **population-mean** temperature or concentration.

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- In the **saline-layer** example, the vertical velocity of the fluid fragments is negative for the heavier and positive for the lighter members of the population.
- Kolmogorov-type models compute **only** population-mean values (although they are sometimes supplemented by **guesses** about the PDFs).
- This is why they simulate combustion processes (for example) inadequately.

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5. How multi-fluid models (MFMs) work

- The working concepts of a multi-fluid model are **few** and **simple.** They are as follows:-

    1. The fluid mixture is regarded as composed of an intermingling **population of individual fluids**, each distinguished by the interval it occupies on the (discretised) PDF abscissa.
    2. A **differential equation** of the standard "conservation" type is solved for the **mass fraction** (i.e. PDF ordinate) of each member of the population; The solutions of these equations provides the PDF for every location and time.

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3. The **source terms** in these equations express:-

    1. the postulated **micro-mixing hypothesis**, which defines:

        a. the frequency with which the different fluids "collide"; and

        b. the re-distribution of material between population members which ensues;

        and

    2. the **speed of movement** of material **in "population space"**, as when a heat source shifts material from low-temperature intervals into higher-temperature ones.

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4. **Additional equations**, either differential or algebraic, are also solved for **non-discretised dependent variables**, for example the velocity components of the distinct fluids, each of which will ordinarily have a different density and so be subject to different body forces.

- Such operations of course increase computer times as compared with those required for Kolmogorov-type models; but the increases are not exorbitant (See below for an example).

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- One-dimensional PDFs (discretized) look like this or this or this. [Left-hand diagram only]

  In these pictures, the left-hand half gives the PDF; the right-hand half is merely a reminder of the "inter-mingling fluid" concept.

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- Populations of fluids may be **multi-dimensional**. Examples of **two-dimensional** populations would be:-
  - the use of:
    1. temperature and
    2. salinity

    for simulating the turbulent-mixing and un-mixing processes described in section 3 above; and
  - the use of:
    1. fuel/air ratio and
    2. completeness of reaction

    for simulating the flow and combustion of turbulent gases in a combustion chamber.

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- A discretised two-dimensional PDF looks like this, or this.

- Examples of **three-dimensional** populations would be:

  - the discretization of all three velocity components for the detailed simulation of turbulent hydrodynamics; and

  - the use of **fragment size** as a third population dimension when temperature and salinity are the other two.

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- It is important to recognise that **the modeller can choose** freely:-
  a. **which** dependent variables to discretise and which to allow to vary continuously for each fluid; and
  b. **how finely** to discretise.

- These choices can be made with the aid of:
  a. **physical insight** into what variables are of dominant importance; and
  b. **population-refinement** studies of essentially the same nature as are used to determine how finely it is necessary to sub-divide space and time.

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  Example 3: how many fluids are needed for accuracy when predicting smoke generation

- These choices may differ from place to place and from time to time. MFM allows the possibility of using **"un-structured"** and **"adaptive"** population grids.

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- It should also be understood that **MFM models can be combined with enlarged-viscosity models**.

- Thus it is common to use the k-epsilon model for the hydrodynamics when the phenomena of greater interest involve chemical reaction or radiation.

- During the oral presentation of the present lecture, examples will be shown of the applications of multi-fluid modelling to:-
  - Example 4: Smoke generation in gas-turbine combustors; and
  - Example 5: Chemical reaction in a paddle-stirred reactor;

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6. Calibrating MFMs

- Multi-fluid models, like those of Kolmogorov type, have ***a priori*-unknown constants** and functions in their equations, the values and forms of which must be **deduced from experimental data**.

- It is possible to use the same measurements as have been used for calibrating the EV-type models, for example the rates of spread of, and the profiles of velocity and temperature in, **turbulent jets, wakes and plumes**.

- However, these provide only indirect evidence of the crucial quantities.

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- More direct evidence is provided by (difficult-to-make) **measurements of the PDFs** themselves. At present, **there are too few such data in the literature**; and these pertain almost entirely to one-dimensional populations.

- It is therefore important to **devise new experiments** which are:
  a. easy to perform, and
  b. rather directly indicative of the micro-mixing process.

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- The so-called **"puff-jet" experiment**, which possesses these qualities, will now be described:
  - A jet of fluid containing a small proportion of chemically-reactive species A is injected steadily into a reservoir containing the same fluid.

  - Then, **for a short period of time**, a small amount of a second species B is injected at the jet orifice, at a rate which is too small to affect the flow field.

  - A and B react as, swiftly as they are allowed by the micro-mixing process, to form a third species C, which species **emits or reflects light**, with the result that a visible (perhaps coloured) cloud of material is seen to move downstream, as indicated below.

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```
                                                  .
   stream of reactant A =====>     .
                                           .
                         .      /////////
_______      .                       /////////////   visible cloud of C
       |                                  ////////////////
- ------ - ------ - ------ - ---- /////////////////
_______|                                  /////////////
       ^ .                           /////////////
       |         .      /////////
       ^                               .
       |                                       .
       nozzle where B was briefly injected, followed by A again
```

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- Since, if there were **no** micro mixing there would be **no coloured-light emission**, and if **micromixing were intense** there would be **maximum emission**, measurement of the amount of the **actual** emission allows the micro-mixing rate to be determined.
- The **shape**, and **speed of motion** of the cloud, will also provide hypothesis-testing information.
- Such experiments will be undertaken at South Bank University, London, in the near future, with ammonium chloride and hydrochloric acid as the reactants in the first instance.
- Switching to liquid reagents will allow Prandtl/Schmidt-number effects to be investigated.

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  - The results of corresponding MFM simulations will be shown during the oral presentation.
  - Example 6: Puff-jet simulations

- If time permits, results pertaining to the simulation of a plane mixing layer will also be shown.

  Example 7: A mixing-layer simulation

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7. Extending MFMs

- Whereas the research on Kolmogorov-type models has been conducted extensively, throughout the world, since the late 1960s, that on multi-fluid models has scarcely started.

- **Opportunities exist** therefore for the further development of such models in several directions, including:-

  a. **experimental**, devoted to devising situations like that of the "puff-jet" which throw light on the postulated micro-mixing mechanisms;

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b. **conceptual**, conceiving **new formulae** for say:

- the influences of Prandtl and Schmidt numbers on the micro-mixing rates;
- the rates of **fragment-size increase** as a result of collision and **diminution** as a consequence of mean-flow shear;
- the **'scattering'** into the y- and z-direction-velocity intervals which results when fragments having differing x-direction velocities collide;

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c. **mathematical**, especially in the development of the creating and handling of un-structured and adaptive "population grids", which:

- use different numbers of fluids (ie abscissa intervals) at different positions and times,
- vary these as the calculation proceeds, guided by optimization rules for:
  1. economy and
  2. accuracy;

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d. **presentational**, so enabling the still-unfamiliar MFM concepts to be grasped by those who can benefit from them, for example by providing:-

    - means of displaying the development of the PDF shapes as the calculation proceeds;
    - applications to familiar flow, heat-transfer and chemical-reaction systems which will reveal how multi-fluid models agree with conventional models where the latter are valid, but with experimental data whare the latter do not;
    - tutorials and self-study material.

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e. **Application-oriented**, because, although much research is desirable, there is **no need to delay use** of MFMs in engineering practice until it has been completed.

    The reason is that such tests as have already been conducted have confirmed the **inherent plausibility** of the multi-fluid approach; whereas to rely on models which **neglect** the intermingled-fragments aspect of turbulence is **inherently unsafe**.

    The k-epsilon and eddy-break-up models were adopted by industry on the basis of much flimsier evidence than now exist for MFM; but **someone had to be the first.**

    Who will be the MFM-application pioneer?

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8. Distinguishing MFMs from other models

- The division of turbulence models into just two types cannot of course do justice to the rich variety of turbulence models which have been invented. It is therefore proper to make a few further explanatory remarks, as follows.

- Multi-fluid models have much in common with, but are distinct from, the **"PDF-transport" models** deriving from the work of Dopazo and O'Brien (1974) and Pope (1982). Because the latter employ a Monte Carlo method of solution, they appear to lack some conceptual and practical advantages which the "discretised-PDF" nature of MFM offers.

  However, given unlimited computer time and care to employ precisely the same micro-mixing formulae, MFM and PDF-transport should produce the same answers.

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- There exist Kolmogorov-type models which do **not** employ the enlarged-viscosity idea. These are the Reynolds-stress models which have been proposed and employed by many workers, for example Launder. Reece and Rodi (1975).

  They still however attempt to deduce all interesting phenomena from the distributions of **statistical quantities**, from which the needed PDFs can **not** be derived.

  No Reynolds-Stress model could predict the "un-mixing" behaviour reported in section 3.

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- Finally **direct numerical simulation** should be mentioned, not because DNS is a turbulence model but in order to lead to the following remark:

  Whereas DNS has sometimes been used as means of deriving the constants and functions of Kolmogorov-type models, it could now equally well be used for testing and augmenting the micro-mixing hypotheses of MFM.

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9. Conclusions

The argument presented in the foregoing lecture will now be summarised, as follows:

a. Of the two main approaches to turbulence modelling, namely
   - Boussinesq-Kolmogorov (i.e. "enlarged-viscosity") and
   - Reynolds-Prandtl (i.e. "intermingling-fragments"),

   it is **the second** which is better able to represent physical reality.

b. Reynolds-Stress models, although they do not use the Boussinesq enlarged-viscosity notion, are no better able to provide the needed PDFs.

c. PDF-transport models based upon Monte Carlo methods, although directed at the right target, have built-in limitations which will continue to prevent their widespread use.

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d. Because of:
   - the attractiveness of Kolmogorov's guess that statistical quantities might suffice, coupled with
   - the limited computing power available when CFD first started,

   Reynolds' intermingling-fragments approach to turbulence has been almost entirely neglected.

e. Now, however, **computing power is more than adequate**; and sufficient work has been done to demonstrate its practicability and promise.

f. The author recommends that approach, as currently embodied in MFM, as the better basis for CFD in the Twenty-First Century.

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10. References

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Turbulence-modelling high-lights through four half-centuries

- **Nineteenth century, second half**

  1. Boussinesq (1877) proposes the "enlarged-viscosity" approach:
     "A turbulent fluid is like a thick soup"

  2. Reynolds (1874) introduces the "inter-mingling-fragments" approach:
     "A turbulent fluid is more like a stew"

     (They did not actually use those words)

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- **Twentieth century, first half**
  1. Prandtl (1925) **uses** the "inter-mingling-fragments" approach (for his "mixing-length hypothesis"), but, for want of other mathematical tools, **casts the result** in "enlarged-viscosity" terms.

  2. Kolmogorov (1942) pays no attention to intermingling fragments at all, but devises the first means for **computing the viscosity enlargement** from transport equations for turbulence and frequency.

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- **Twentieth century, second half**

  1. The primitive computers of the late '60s and early '70s enable workers in Los Alamos, Imperial College and elsewhere to devise software which **solves the transport equations**; so **CFD is born**.

  2. CFD-for-**combustion** specialists are forced to adopt the "intermingling" fragments approach in order to fit the facts.

  3. CFD-for-**multi-phase-flow** specialists show how **the multi-fluid transport equations can be solved** .

  4. Computers increase in power; but most turbulence modellers continue to use power-restricted concepts.

  5. Nevertheless the first steps are taken to develop **multi-fluid models** which make use of **both** the Boussinesq and Reynolds concepts.

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- **Twenty-first century, first half**

  1. October, 2000: Audiences in Beijing and Shanghai are presented with the argument that, since:
     a. more than adequate computing power is now widely available,
     b. already one general-purpose CFD code (which can be accessed via Internet) has MFM built into it,
     c. the superior plausibility of MFM for many processes has already been demonstrated,

     it is time at last to switch from Boussinesq to Reynolds.

  2. Thereafter, ?????

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Links to explanations of the micro-mixing hypothesis of MFM

- Parents and offspring

- Brief encounters
  - A 1950 analysis
  - Scalar transport; or energy dissipation
    - High Reynolds number
    - Low Reynolds number
  - Diffusion and heat conduction with chemical reaction
    - High Reynolds number
    - Low Reynolds number

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