

# Benjamin Franklin & CFD; introduction

### April 2010

Fluids played a large part in the life of Benjamin Franklin.

- As a boy, he wanted to be a sailor;
- but his father was a 'Tallow Chandler'; so he had to melt **tallow** and pour it into moulds to make candles.
- Later apprenticed to his printer brother, he adopted **printer's ink** as his career fluid.
- He was a good swimmer; and when he absconded to Philadelphia, he travelled by **water**, spending much time **immersed in** it.
- And when he arrived it was raining!

In his middle age he became affluent enough to indulge his **inventive talents**; then it was with **gases** that he was concerned, especially in **lamps** and **stoves**.

In this lecture I speculate about how he might be **exploiting CFD**, were he alive today.





# Benjamin Franklin & CFD; introduction

- In 1774, Benjamin Franklin sailed for England on a ship which its captain had claimed to be swift. But it proved not to be.
- So all passengers were called on deck and ordered, with the crew, to huddle in the stern.
- Then the ship 'mended her pace'; I from which it was concluded that the cargo had been badly distributed.

Franklin remarked on the **lack of coordination** between the **hull** designers, the **sail and rigging** makers, those who distribute the **cargo**, and the sailors who **trim the sails**; and added: "I think that a set of **experiments** might be instituted, to determine the proper form of the hull..... The Properest Place for the Mast ... Form & Quantity of Sail..." and so on.

Indeed he was sure that "some **ingenious philosopher** will undertake it; -- to whom I wish Success".

Had CFD existed then, he might well himself have been that 'philosopher'.



# CFD and sailing

CPHOTON

Vector 0.33

0.40 0.42 0.44 0.46 0.48 0.50 0.52 0.54 0.55 0.57 0.59 XY

V-

CFD has indeed made contributions to sailing-ship design; and my colleague Gordon Mallinson can claim some credit for New Zealand's sailing successes of the late 1990s.



The sail in a **physical** wind-tunnel

The sail in a virtual wind-tunnel

Min: 3.28E-01 Max: 5.92E-01

3.00E-01

BFC 3D SPINNAKER

Most CFD specialists will regard such studies as commonplace; but my next example concerns something less well-known: the '**deadwater effect**' which puzzled such explorers as **Fridtjof Nansen**.



#### CFD and the 'dead-water' effect

#### April 2010

#### Dead water

"dödvand": Norwegian mariner's term sudden, severe slow-down of a ship as though an anchor has been dropped or the ship has grounded.

#### The surface

has a glassy look surrounded by turbid edges; is sometimes accompanied by a prolonged hissing sound which follows the ship over a wide area; and the ship becomes hard to steer.





#### CFD and the dead-water effect

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Nansen's observations, 1893-1896 North-Polar expedition with the *FRAM*:

"...moving at 5 knots, when the speed suddenly dropped to 1 knot and stayed that way." "We swept the whole sea along with us..." "The moment the engine stopped, it seemed as if the ship

was sucked back."



Ekman (1904) provided the explanation; the presence of **density stratification** causes the ship to generate energy-consuming gravity waves. h



Nansen



FRAM

Ekman



CFD and the dead-water effect; the Maas-Hornby investigation

#### April 2010

The dead-water effect has been simulated in **small-scale laboratory** experiments by Dr LRM Maas of the Netherlands Sea Research Institute, Model'ship



and in **3D transient CFD** calculations by Dr Bob Hornby in the UK.

The **agreement** between experiments and calculations was **excellent**, as of course it should be; for **turbulence** played no **significant role**.



I think that Benjamin Franklin would have admired this investigation; for it possesses what he called '*a certain charming quality....* **SIMPLICITY**'.



Combustion, turbulence and CFD; Benjamin Frankln's contributions

## April 2010

One of Benjamin Franklin's many interests was **combustion**, both scientific and practical. He corresponded with Joseph **Priestley**, the English discoverer of **oxygen** (the Swede **Scheele** did so earlier); and he watched Antoine **Lavoisier** demonstrate charcoal burning in '**de-phlogisticated**' air.







On the practical side, he invented an improved **oilburning** lamp; for he had seen that the earlier globeshaped lamp allowed too little air to enter and so became quickly blackened by smoke. **His** lantern's plane-glass sides **facilitated** air entry; and so remained clean.

The flows of **air**, **heat** and **combustion products**, were his main concerns when he urged replacing open **fire-places**, which lost much heat to the outside wall, by a **stove in the centre** of the room.

I follow Franklin by bringing combustion into the centre **of the CFD stage**; for it can teach us much.





Combustion, turbulence and CFD; the population analogy

#### April 2010

There are **two reasons** why CFD specialists should pay attention to **chemically-reacting** flows:

 without them there would be no engines, furnaces or chemical plant to generate the chemically-inert flows to which attention is paid; and
 their study provides unique insight into turbulence which affects all flows.

Let us now ask ourselves **what Benjamin Franklin would notice** about turbulent flames if he came back to advise us.

I suggest that he would be struck by their obvious intermittency. At any one location, there may be sometimes pure air, sometimes pure fuel, and most of the time fragments of gas with intermediate fuel-air ratio and degree of reaction.

Remembering how 'savages' and colonists so often changed places, he might have used the '**population analogy**' to describe flames.





## The Population Analogy

#### April 2010





Combustion, turbulence and CFD; the population analogy (continued)

#### April 2010

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Benjamin Franklin was a **methodical man**, and he liked to express his ideas **graphically**.

I. On the right, for example, is how he recorded each of his lapses from the strict moral standards which he required of himself.





I therefore imagine that he might have devised a **two-dimensional** diagram so as to represent instructively the **population of gas states**, members of which might be found in a combustion chamber.

It could have taken the triangular form on the left, with vertices representing pure **air**, **fuel** and **combustion products**, respectively, with all possible gas states, *i.e.* **population members**, **between** them.



Combustion, turbulence and CFD; the population analogy (continued)

#### April 2010

fuel

products (hot)

(cold)

He might have called this the **TRI-MIX** diagram because:

- its ordinate is the Temperature **RI**se which would result from adiabatic combustion;
- its abscissa is the **MIX**ture fraction of material derived from the fuel stream *(i.e.* loosely, the **fuel-air ratio**).

On the right it displays the **contours of population distribution** for a **particular location** in a flame.

The diagram can also be used to:

- to show how population properties depend on the co-ordinates; and
- to describe and explain the various **hypotheses** which scientists have used so as to represent flames, when using the techniques of CFD.

I shall illustrate both of these uses in the next slides.



Some uses of the TR-MIX diagram; mixture properties

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Our Returned Benjamin Franklin (RBF from now on) will certainly want to visualize the **composition** of the gas population in its possible states.



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

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

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



PHOTO



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



Some uses of the TRI-MIX diagram; chemical-reaction rates

#### April 2010



**Svante Arrhenius**, 100 years after Priestley and Lavoisier, explained why combustion reactions proceed **fastest at high temperatures**. His findings can also be expressed by way of **contours on the TRI-MIX** diagram.

There are **three kinds** of reaction, 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 almost equally undesired **smoke-creating** reaction (although **light** emanating from Franklin's oil lamp **does** need the presence of **some** carbon particles).



2.4E-5 5.3E-5 7.9E-5 1.1E-4 1.3E-4 1.4E-4 1.4E-4 2.4E-4 2.4E-4 2.4E-4 3.2E-4 3.4E-4 3.7E-4



Some uses of the TRIMIX diagram; combustor-design strategy

#### April 2010

Once he had completed his diagram, RBF, being still a sailor at heart, would have immediately conceived the optimum **combustor-design strategy** in the form of a voyage.

The good ships **Primary Air** and **Fuel** rendezvous in cool waters.

They then proceed in convoy towards and beyond the **fastestoxidation region**, avoiding **Scylla**-NOX to larboard and **Charybdis**-Smoke to starboard.

Then, their crews being totally intermingled, they set first a southerly and then, having met **Secondary Air**, westerly course, arriving at their **Out** port with minimum pollution.





Some uses of the TRI-MIX diagram; Franklin's ideal gas-turbine combustor

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This is how his ideal design for a gas-turbine combustor might have looked, with **three distinct parts**:



The final dilution must be **very rapid** so as to minimise NOX.



Some uses of the TRI-MIX diagram; combustor-design strategy

#### April 2010

Were Benjamin to impart his ideas to designers of **gas-turbine** combustor, he would be told: "**That's just what we do**:

- the fuel and primary air mix and burn in the upstream part of the chamber;
- downstream, the **secondary air** enters so as to lower the temperature to that which the turbine blades can stand."



**RBF**: "Hmmm! But how do you optimize **sizes** and **positions** of holes?" **Specialist**: "**We use CFD** for that."

RBF:" What's CFD?"

**Specialist**: "Computer simulation. It applies **conservation laws** of mass, species, momentum and energy to a '**grid**' of **finite volumes** in space and time.

Then it solves the equations so generated by trial-and-error."



Some uses of the TRI-MIX diagram; what CFD does and doesn't do

#### April 2010

Fuel



Benjamin would have understood instantly that: CFD requires only the **skills of the storekeeper**, to count:

- what comes into each volume,
- what goes out, and
- what is created or destroyed there;

for he sold newspapers in his shop; and he studied 'Cocker's Arithmetick with great Ease'. Moreover **Trial-and-Error** was a way of life for colonists of a new territory.

Ai

**RBF**: So I suppose you do the **same thing for the gas-population** distribution? (expecting to be shown some such '**grid**' as that on the right.)

#### **Specialist: What's a gas population?**



Some uses of the TRI-MIX diagram; what CFD does and doesn't do

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**RBF** (surprised): The Temperature RIse and MIXture fraction dimensions. Are they not discretized as well?

**Specialist** (puzzled): I never heard of that. We just use Ansys like everyone else.

**RBF**: But what about turbulent fluctuations of temperature and fuel/air ratio?

**Specialist**: I quess we take the **time-average** temperature; and fuel-air ratio as well.

**RBF**: But if you calculated **what proportion of time** the local gas state was in **each cell** of the **TRI-MIX** diagram, could you not make **better estimates** of the rates of **combustion**; and of **NOX**; and of **smoke**?

Specialist: Yes; I suppose so; but how?











Some uses of the TRI-MIX diagram; a Socratic dialogue

#### April 2010

When he was young, Benjamin Franklin consciously copied Socrates;  $\Rightarrow$  so, by **artful questioning**, RBF might have led our 'how-'asking specialist finally to understand and **admit that**:

- There is no essential difference between distributions in geometric space and in population space.
- The **same** techniques (discretization, balance equations, trial-and-error **solution**) can be therefore be used for **both** spaces.
- Sometimes (*e.g.* in well-stirred regions), non-uniformities in **population** space are **much more important** than those in **geometric** space.
- To use, say, a **million geometric-space** sub-divisions but a single **population** one **perhaps** (mild-spoken Franklin might say) lacks balance.
- **How many** sub-divisions to use in each space is best decided by trying several and observing the difference in the results.
- Provided CFD's current **over-simplification** is not replaced by **needless over-complication**, computation-time expense will increase but modestly.



# Geometric and population grids compared

#### April 2010

Brow-beaten by Socratic questioning, our specialist has assented to RBF's propositions. **My** audience however may require **more time**; and indeed **motivation**.

 I address first those interested only in velocity and its fluctuations, *e.g.* in a boundary layer on a curved wall.



• These fluctuations can be described by a **one**-dimensional **population**, with **w** as the independent variable. Its distribution, **calculated as will be explained**, shows how centrifugal force 'filters' larger-w elements outwards; so **swirling flows** are simulated **realistically**.

• Likewise 'gustiness', which affects both human comfort and windturbine safety, can be expressed *via* the w-population distribution.

• 2D populations of hydrodynamic interest have **temperature** and **salinity** as independent variables. They are needed for simulation of dead-waterlike **gravity waves** when thermal and saltiness stratification co-exist.

• Now, back to **combustion**.



#### Geometric and population grids: 3D plus 2D = 5D (but it's not that bad)

#### April 2010



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.



Geometric and population grids: physical and chemical processes involved

### April 2010



Neighbouring cells of the **geometric grid** influence each other by way of: **laminar and turbulent diffusion** and **convection**; **pressure gradient and body forces are also active**.

**Differential convection**' ('filtration', see later) can also play its part.

Neighbouring cells of the **population grid** influence each other by **chemical transformation** (similar to convection) and **engulfment** (without geometric counterpart) to be described below.

Each element of the population can also, if desired, have its own additional variables (*e.g.* NOX concentration); but **don't over-complicate**!



Interactions between members of the population at one cell in the 3D grid

#### April 2010

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#### Interactions between population members; the engulfment hypothesis

## April 2010









Countless numerical and experimental studies reveal the prevalence of vortex **roll-up** in turbulent flows. **1** 

It results, when two recognisably different fluids lie close together, in their '**engulfing**' each other, as shown on the right.



Their interface becomes **stretched**; and the thickness of the inter-leaved layers becomes **thinner**, so that laminar diffusion and heat conduction **per unit volume** increase enormously.

Underlying turbulent shear may thus cause population-element mingling.



#### A feature of populations only: differential convection or 'filtering'

#### April 2010

Although it is **nearly** true that all population elements are convected together, there are exceptions, as Benjamin Franklin will have known.

- Red Indians can **run and ride faster** than colonists; and they often attack what the latter flee from.
- In combustion chambers, pressure gradients cause hot to accelerate more rapidly than colder ones.



• In lecture rooms, hot air rises even though the air near the cells already hotter. It is a kind of 'filtering' of one fluid through another.

• In flow along a curved wall, faster-moving fluid fragments migrate to the larger radii, slower-moving ones to the smaller. [Swirling flows cannot be understood if this is not allowed for. It is a population-distribution matter].

- Mathematical expressions must therefore be devised, and calibrated, to represent the various possible 'filtering' processes such as the above.
- Similar problems arise in 'sedimentation', familiar in multi-phase flow'.



# Geometric and population grids; what's new?

Does CFD recognise the population dimension, perhaps in other words?

**Yes**; the 1971 '**eddy-break-up model**' (EBU) for combustion simulation did so, postulating a **two**-member population: *viz.* **burned** and **un**burned. The rate of inter-mingling was precisely the **engulfment** rate.



It solved the 'Scurlock puzzle', *viz*. **why** did the turbulent- flame angle **vary little** with: **inlet** velocity, fuel-air ratio, temperature, *etc*.?

The EBU is represented on TRI-MIX by **red** squares and joining line. Engulfment products **burn at once**.

The EBU model is **still in** (indirect) **use**; so the engulfment-rate concept has, **with empirical constant**, been (tacitly) accepted.





Geometric and population grids; Other tentative steps into population space

### April 2010



A 1982 **'two-fluid** ' model of transition to detonation has shown how hotter population elements (right) are accelerated faster than colder elements (left).



Variants of EBU, namely:

- eddy-dissipation concept,
- presumed-pdf,
- 'flamelet')

have adherents;

but none have recognised the need to calculate the **distribution throughout** TRI-MIX space.





Geometric and population grids; More serious steps into population space

#### April 2010

Pope's '**pdf-transport**' **model** employs a Monte-Carlo method to 'populate' a (usually) 1D representation of possible gas-mixture states in a combustor by 'particles' having different composition.

It is rarely used by designers, perhaps because of computational expense.

Proportion of box which is filled indicates proportion of mixture in relevant state



<-- state of one of the two entering streams, viz hot combustion products plus additional fuel

Vertical scale represents the proportion of the fuel for which sufficient oxygen is available which has already been burned The author's '**multi-fluid model**' corresponds quite closely to RBF's Ideas; but, being devised before the TRI-MIX diagram was invented, its results-display methods (see left) may have hindered acceptance.

Nevertheless, the **triangular** region of occupancy is discernible in the image on the left.



More about the 'multi-fluid' model (MFM): origin, name and applications

### April 2010

MFM was born in 1995, so as to extend the **2-member-population** EBU to a **4-member** one. This was used for **oil-platform** explosions; but soon generalised.



The (perhaps **ill-chosen**) **name**, '**multi-fluid**', means only that each member of the population is called a 'fluid', for want of a better word. Each such 'fluid' is a **figment of imagination**, no more real than the cells into which the CFD specialist divides geometric **space**.

Although arising from combustion studies, MFM has **more general utility**. I conclude therefore by showing two **non-combustion** applications, both involving **one-dimensional** populations. They concern:

A stirred chemical reactor;



and flow in a curved duct.





Application of MFM to a stirred chemical reactor

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Here is an old CFD-benchmark problem: 3D, transient with a rotating central paddle. We consider the **mixing** and rapid reaction of **acid**, in the bottom half, with **alkali** in the top half. The geometric grid is shown below.





Two cases are considered, 1. **neglecting** and 2. **considering** population effects.

For case 2, the acid~alkali range is divided into eleven equal parts

Case 1 is what most designers use today; but it is too optimistic.



Application of MFM to a stirred chemical reactor: conclusion

#### April 2010

3D contour diagrams of product concentration **after 10 paddle revolutions** are shown for **cases 1 and 2**.

The general patterns differ little but their quantitative scales **do**: namely from **3.2 to 2.4**. **So neglecting fluctuations over-estimates reactor performance**.





The **explanation** lies in the following calculated **mixture-ratio histograms**, corresponding to a single: instant of time, vertical height and circumferential angle, at six different radial locations.



Product concentration is high only for the middle mixture ratios.



Extract from a Moscow-2008 lecture on swirl-flow simulation illustrating 'filtering'



#### April 2010

- 1. The general-purpose CFD code 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



4. Turbulent-diffusion/engulfment-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 'filtering hypothesis' was formulated.

This was based on 'drift-flux' and 'algebraic-slip' concepts already **long** used in two-phase-flow simulations.

The computations, of which a few results will be displayed, employed only standard features of PHOENICS.



Extract from a Moscow-2008 lecture: swirl-flow simulation, illustrating 'filtering': fluid-concentration contours

April 2010

First: **zero curvature**, *i.e.* **no** swirl.; **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.

Next, contours for the **9<sup>th</sup> fluid** with velocity equal to the mean wall velocity. They spread as a consequence of turbulent **diffusion opposed by population-member mingling**. Downstream cessation of spread implies that the two processes are **in balance**.

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

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





#### Extract from a Moscow-2008 lecture: swirl-flow simulation; the effect of 'filtering' on velocity FDP's

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0.000

0.013

0.027 0.040

0.053 0.067 0.080

0.093

0.120 0.133 0.147 0.160 0.173

0.187

0.00 0.01 0.03

0.04

0.07 0.09 0.10

0.12 0.13 0.15 0.16

0.18 0.19 0.21

FPD 0.000

0.006

0.017 0.023 0.029 0.035 0.041

0.046 0.052

0.058 0.064 0.070

0.075

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 average **velocity increasing with radius**; the distribution becomes **narrower**. The **fluid-9 mass fraction has risen** to 0.21. Faster fluids **filter** towards **the faster-moving outer wall**; and the **shear stress de**creases.

Now the **direction of curvature is reversed**. Faster-moving fluids now **filter away from** the faster-moving **inner** wall. The shape of the FPD **broadens** dramatically. **Fluid-9 mass fraction has fallen** to 0.081; and the shear stress **in**creases.

These results explain why flows near **convex** and concave walls are so **different**. Only **population models** can begin to simulate **swirling- flow behaviour.** Should they not be **investigated**?



Concluding remarks: 1. What may be deduced from the examples just shown

## April 2010

To those for whom the population-grid idea was new, three rejection-prompting thoughts will surely have occurred, *viz.*1. It concerns combustion, a special subject of little general interest.
2. Its ramifications appear vast and indefinite, requiring immense resources of computer- and man-power for its exploitation.
3. To the familiar menagerie of convection, diffusion and time-dependence, there have been added new animals called 'engulfment' and 'filtering', which may not 'get along with' the others at all.
The examples have therefore been chosen to show:
That non-combustion phenomena involving the flow of air (swirl)

- That non-combustion phenomena involving the flow of air (swirl, gusts), which elude conventional turbulence models, positively necessitate population-type analysis.
- 2. That **no vast** resources are required. A few individuals with **lap-top** computers and modest mathematical skills have already done much.

3. The engulfment and filtering concepts have been in use for **decades**.

What is however **not** claimed is that anything more than **pioneer settlements** have been planted in the new territory. Hordes of industrious **new immigrants** are needed to exploit it.





### Concluding remarks 2. About the population aspects of CFD

- I hope to have convinced you that RBF's immediate recognition of the **analogy between geometric** and **population distribution** was correct.
- I have also argued that understandable apprehensions concerning its difficulty of implementation are groundless.
- The question I now pose is therefore: **why should we not** give the **latter** as much attention as the **former**, at least for chemically-reacting flows?
- And not for them only; for pure-hydrodynamics problems have their (1D- or 2D-) population aspects which required investigation?
- We can choose the population-defining attributes (replacing the above TRI, MIX, w, acid/salt ratio and salinity,) to suit our purposes. • Particle size' would be important in 'volcanic-ash-and-aircraft' simulations.
- MFM as described here 'rides on the back' of k-epsilon for hydrodynamics; but a **stand-alone MFM** might be created using, say, '**shear-rate**' and '**eddy-size**' as population-defining attributes.
- The general conclusion is: we still have as much **intellectual** territory to explore as Franklin's contemporaries had **geographical**.



# Concluding remarks 3. A final question

#### April 2010

But perhaps I have **not** convinced; and, if that is the case, I sincerely ask: **How did I not**? Truly wanting to know. For it would not be the first time. Was the argument not clear? Or is the population concept hard to grasp? Or was there something else?

Benjamin Franklin wrote about his own experiences as a persuader: The objections & reluctances I met with ... made me soon feel the Impropriety of presenting one's self as the Proposer of any useful Project .... I therefore put myself as much as possible out of sight and stated it as a Scheme of a Number of Friends..... In this way my affair went on very smoothly, and ..... I can heartily recommend it."

Henceforth I shall follow his advice. That is why I presented the **population-geometry analogy** as being **his** idea rather than mine.

**So** let it remain in **your memories**; and when you talk about it to others, please be **my** 'Friends'. Then **this** idea also may spread more smoothly.

For this kind service, and for your attention, I offer my sincere thanks.



## Figures to be placed in the word document at appropriate places

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Figures to be placed in the word document at appropriate places

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#### Figures to be placed in the word document at appropriate places

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Up

Air



Figure 10

#### Figure 8

Mix