Brian Spalding and Turbulent Combustion

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1 Introduction

Brian Spalding regarded the simulation of combusting flows as one of the main driving forces behind the emergence of CFD as another tool in the engineer's toolkit:

> It could be reasonably argued that it was the needs of the combustion engineers in the aerospace industry which brought the CFD-software business into existence, the reason being that the complexity of the combustion process left expensive experimentation as the only alternative. [107]

Brian Spalding is well known for his contributions to Engineering and Science in numerous fields, including numerical methods, thermodynamics, turbulence, heat and mass transfer, multiphase and free-surface flows. Combustion featured prominently among the subject matters of Spalding's research writings. A quick survey of his scientific production shows that about 32% of his contributions in his 67-year academic career were directly related to combustion (Fig. 1).

This chapter presents an overview of Spalding's contribution to the modelling and simulation of combustion. In doing so, we attempt to follow his thinking as he progressed from the integral models of the early years to the multi-fluid models of the latter ones. The focus is therefore in finding and conveying his line of thought, rather than in the mathematics or the numerics of the result; the latter can be found in the references cited, and in many others that are not included for reasons of space. We do not attempt, for the same reasons of space, to be encyclopaedic in our account.

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A. Runchal (ed.), *50 Years of CFD in Engineering Sciences*,
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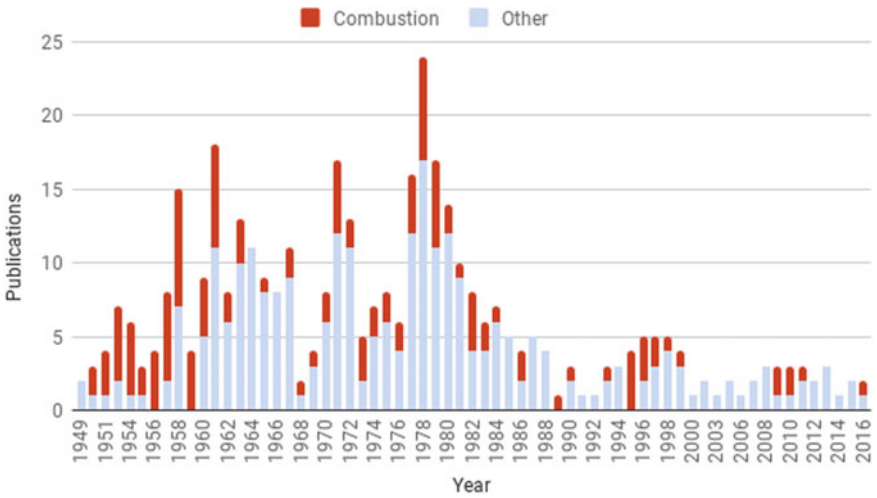

Fig. 1 Spalding's research writings on combustion

Spalding's masterful command of the written language was for many as engaging as the scientific ideas it conveyed. His writings are full of powerful images, literary references, witticisms and flares of plain humour. In this recollection of his contributions to combustion science, we often cite his own words; we signify this by using double quotation marks "⊙", while we reserve single quotation marks '⊙' for all other, non-citation uses.

We reproduce a few of the figures and diagrams that also define Spalding's production, from hand-made graphical depictions of his ideas in the early years to his use of 'ASCII Art' in the latter ones.

The chapter is structured in six sections. After this introduction, in the second section we cover the 'early' years, from his Ph.D. thesis to his first uses of computers. The third one is dedicated to the popular Eddy-Breakup Model, and its (perhaps less popular) sequel the ESCIMO Model. The fourth and fifth sections cover Spalding's most recent thinking on turbulent combustion: the Two- and Multi-Fluid Models of turbulence and combustion. We close the chapter with some conclusions.

2 The Early Years

2.1 The Pre-computer Years

Spalding's scientific interest in the intricate field of combustion dates back to his research leading to his Ph.D. thesis at University of Cambridge, which he concluded in 1951 [81]. The thesis combined Spalding's masterful command of the

theoretical grounds with a set of simple but ingenious experiments. The research addressed the prediction of the rate of combustion from a liquid-fuel surface (a sphere) into a surrounding gas, and presented a rigorous and elegant treatment of the associated, complex heat and mass-transfer phenomena between the liquid phase and the surrounding gas. Spalding studied both "envelope" and "wake" flames, and the "breakdown" of the latter (or their extinction, as it would be more commonly called nowadays). The then-called *Transfer Number* was for the first time presented, and a whole thesis chapter was dedicated to its calculation for several configurations (Chap. 3); this Transfer Number was later called, and is still known as, *Spalding's Number*, *B*. In his preface to a re-typed, 1987 edition version of the thesis [103], he humorously declared to be "pleased to find" that his re-reading it "did not cause me much embarrassment", despite "[some] misplacings of the word 'only' and the omissions of hyphens and commas". (Later in his career, he would try to spare his own students from such predicament by publishing a style booklet entitled 'The Writing of Technical Reports' [96].)

In this pre-computer age, Spalding recognised two important limitations of his theory: first, the need to use constant values for the properties; second, that the gas flow-field had to be analytically prescribed.

It is perhaps this latter one that prompted Spalding to initially explore the use of the then-called analogue *computers*. These were devices used to mimic the behaviour of physical processes, such as heat transfer. Spalding, now at Imperial College, contrived several of these devices to investigate combustion and heat-transfer problems [72]. One of such devices was created for the physical simulation of bluff-body-stabilised flames [82] using heated air (Fig. 2). The 'combustion' chamber consisted in a Cartesian array of heating rods downstream of a baffle. Each rod was equipped with a thermocouple, and the heating element in each rod was turned on or off (manually!) as a function of the local temperature, thus representing the effect of the activation energy on the reaction rate.

The device was successful in predicting 'flame' extinction [82], and the predictions compared reasonably well, given the model limitations, with real-flame experiments. In the subsequent discussion of this paper [82], Owen Saunders (Fellow of the Royal Society 1965) that "an extremely ingenious tool had been devised which brought together the chemistry and physics of combustion in a new way".

Forty years later, reflecting on this piece of research, Spalding recognised [107] that the Cartesian arrangement of the rods was perhaps not unlike the discretisation techniques he would later pioneer; and that he was unaware at the time "of the turbulence-chemistry interaction problem", to which he would dedicate much of his time in later years (see below).

2.2 Spalding 'Goes Digital'

By the early 50s, even before Spalding developed his analogue combustion chamber, the applications of digital computers to combustion science were starting to

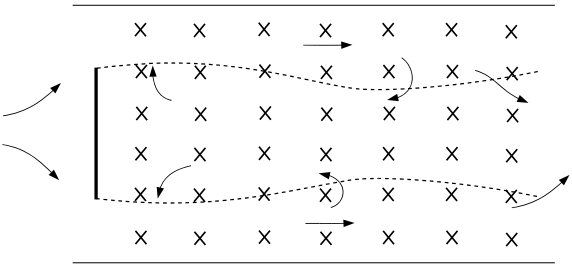

Fig. 2 Schematic of Spalding's 'analogue combustion chamber'. The crosses represent the heating rods; the dashed line represents "the region where the air temperature appreciably exceeds that at inlet" (re-created from [82])

emerge [23]. Spalding's first published use of computers to a combustion problem is perhaps the Adler and Spalding paper where they presented numerical solutions of one-dimensional, laminar, premixed flames with simplified chemistry [1].

Unlike most of the premixed flames studied until then, the focus in this paper was on flames subject to enthalpy gradients; such situations are often encountered in practice when the flame products transfer heat, through conduction or radiation, with the reactor wall or with the surroundings. They concluded that, compared to adiabatic flames, positive enthalpy gradients increased the burning rate, while negative ones decreased it.

The computer used was a Ferranti Mark I*, similar to the one shown in Fig. 3.

2.3 The First CFD Combustion Calculations

The next large stride towards the numerical simulation of combustion was the development of a calculation method for parabolic flows as part of Suhas Patankar's 1967 Ph.D. thesis [59]. The method was, in 1969, used in the GENMIX code [92] to simulate laminar and turbulent jet flames for the first time.

For further progress to be made, a method was needed to remove the parabolic restriction from the problem formulation. Akshai Runchal and Micha Wolfshtein joined Brian Spalding's team of students soon after Patankar to work on elliptic and turbulent flows. As a consequence, the first method for solving elliptic flows was created around 1968 [20]; it was the 'vorticity-stream-function' method, and it would be extensively used for a few years for calculating mainly inert, recirculating flows.

The method used, also for the first time, the concept of 'upwind differencing', the creation of which Spalding famously attributed to "[his] childhood experience of having lived near a pig-sty, and therefore known well how the direction of the wind influenced the strength of the influence of near neighbours" [107].

Soon after the creation of the 'vorticity-stream-function' method, Spalding (together with WM (Sam) Pun) started its application to chemically reacting flows, resulting in 1967 in perhaps the first simulation of a recirculating, reacting flow using

Fig. 3 Ferranti Mark I computer: the console is at the back; the logic circuits are in the cabinets along the sides of the aisle (Courtesy of the University of Manchester, with additional thanks to Prof Jim Miles, School of Computer Science; James Peters, National Archive for the History of Computing; and Fujitsu Services Limited.)

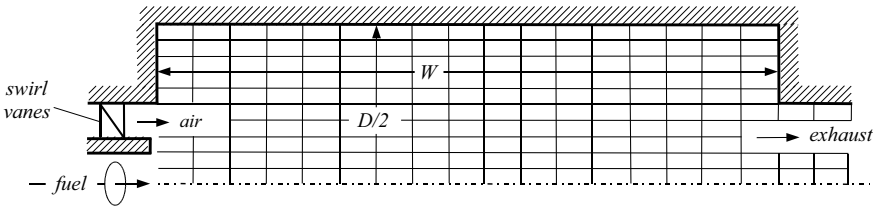

Fig. 4 First elliptic flame calculation: domain and mesh (re-created from [68])

CFD [68]. This work considered the simulation of a non-premixed, swirling flame in a combustion chamber, re-created in Fig. 4 from the original figure in [68].

Turbulence was represented with a simple effective-viscosity model, and combustion with a mixed-is-burned hypothesis based on the Burke–Schumann Simple Chemically Reacting System (SCRS) [87]. The aim of the paper was to demonstrate the feasibility of performing calculations of recirculating, reacting flows. The cal-

culations were performed on an IBM 7090 computer, at a cost of between 2 and 6 minutes per case for a 161-cell mesh.

It was around this time that Spalding [84] began to consider the problem of how to predict a finite thickness for the reaction zone of a turbulent diffusion flame when using an SCRS combustion model based on fast chemistry. The SCRS assumes that fuel and oxidiser cannot coexist at the same location, even at different times; and this leads to a very thin reaction zone, with peaky flame profiles, rather than a thicker flame brush. For more realistic predictions, Spalding [84, 86, 111, 112] recognised the need to account for the fluctuation in mixture strength with time; and hence for the fluctuations in species mass fractions, in temperature and in fluid density, which are often large compared to their mean values.

For this purpose, Spalding devised a modified model in which the reactants cannot exist at the same location at the same time, but can occur at the same location at different times. This was done by assuming a rectangular wave variation of the mixture fraction f with time, and the magnitudes of the fluctuations in f were determined by solving an additional transport equation for its variance. This approach amounts to using an assumed probability density function (PDF) for the mixture fraction in the form of a double-delta function, and it was used later by Gosman and Lockwood [19], Khalil et al. [37] and Serag-Eldin [73]. Other workers soon adopted the method, but to obtain improved results the double-delta function was replaced by more realistic PDF forms, such as the clipped Gaussian or the beta distributions (see Jones and Whitelaw [35]).

2.4 The Gateway to 3D Combustion Calculations

In the fast-paced late 60s and early 70s, the Imperial College group led by Spalding soon came up with what would become the mainstream method for three-dimensional recirculating flows. It was based on the solution of the so-called primitive variables: velocity and pressure. This was an extension of the SIMPLE procedure [62], so far used only for 3D boundary layers, to recirculating flows.

Their landmark 1974 publication [61] about the simulation of a gas-turbine combustion chamber contained all the ingredients needed for three-dimensional CFD modelling of combustion. (However, Spalding credits Zuber [131] as the creator of the first 3D chamber model in 1972.) Patankar and Spalding's model used SIMPLE for solving the velocity–pressure coupling; the $k - \epsilon$ model for turbulence; a six-flux radiation model [60]; and a single-step, equilibrium model for the chemical reaction.

This pioneering method would be soon afterwards exploited by Spalding's student Amr Serag-Eldin. His 1977 Ph.D. thesis [73] would highlight, through the comparison of calculations and experiments, the many deficiencies of the physical models available at the time for combustion CFD modelling. Among these, the need was clearly seen for modelling the interaction between turbulence and chemistry, and the effect of chemical kinetics. Spalding would dedicate a significant fraction of his academic career to redress such deficiencies.

3 EBU and ESCIMO

3.1 The Eddy-Breakup Model

Spalding's most recognisable contribution to combustion is arguably his Eddy-Breakup (EBU) model. (There is ample documented evidence that Spalding thought this model too long-lived, as we will discuss below.)

In its original form, the EBU model was first published in 1971 [112]. Spalding was researching the reasons why the spread angle in confined, premixed, turbulent flames was nearly independent of the operating conditions, including the unburned mixture velocity, its composition, its temperature or its level of turbulence. The hypothesis that the fresh mixture burned immediately following entrainment into the burnt gases had already been made, and Spalding noted that he had tested it numerically [83], and found that, although it "could fairly well explain the observed phenomena", his validation against experiments showed that "the assumption [was] far too crude" and that unburned fuel could be found even well inside the flame.

While Spalding's first approach to the problem in 1967 [83] had used an integral formulation, he now had at his disposal powerful new tools: computational methods to solve, via discretisation, partial differential equations in parabolic flows; and increasingly sophisticated models for the turbulence energy and its length scale.

The original EBU model was formulated in terms of the reactedness variable τ:

$$\tau = \frac{m_\mathrm{f} - m_\mathrm{f,unburned}}{m_\mathrm{f,burned} - m_\mathrm{f,unburned}} \quad , \tag{1}$$

where m_f is the local value of the mass fraction of fuel.

From its definition τ can be regarded as a non-dimensional fuel mass fraction.

Central to the EBU model, and to Spalding's view of turbulent combustion, is the supposition that "the mixture is mainly composed of alternating fragments of unburned gas and almost-fully burned gas" (and thus largely non reactive), and that it is "at the interfaces between the hot and cold lumps", with intermediate compositions, where combustion takes place, with a maximum reaction rate (per unit volume) of, say, $\dot{m}_\mathrm{max}$. Spalding then further argued that the breaking down of these parcels into increasingly small ones (down to the Kolmogorov scale) is the cause of turbulence decay; and that the decay rate, for turbulence in equilibrium, is proportional to the density and velocity gradient, i.e. equal to $0.35\rho\,|\partial\overline{u}/\partial y|$, where $\overline{u}$ is the average velocity.

From this, he assumed that the breakdown of parcels into sufficiently small ones for heat conduction and chemical reaction to be significant proceeds at the same rate, and thus is (in terms of mass per unit volume per unit time):

$$\dot{m}_\mathrm{mix} = C(1-\tau)\rho\left|\frac{\partial\overline{u}}{\partial y}\right| \quad , \tag{2}$$

which is the essence of the Eddy-Breakup model.

It is interesting to note that in this first version Spalding included the influence of the kinetic rate, crudely represented by a conversion rate (mass per unit volume per unit time):

$$\dot{m}_{\text{kin}} = \tau \dot{m}_{\text{max}} \quad , \tag{3}$$

so that the effective reaction rate is a harmonic blend of both the kinetic and the mixing rates, thus ensuring that the overall rate is dictated by the slower process:

$$\dot{m}_{\tau} = \left[\frac{1}{\dot{m}_{\text{kin}}} + \frac{1}{\dot{m}_{\text{mix}}} \right] \quad . \tag{4}$$

At the time, more sophisticated turbulence closure models were being developed that allowed for the transport of turbulence statistics, thus dispensing with the hypothesis of local equilibrium. Spalding was at the time exploring one of these models, namely, the $k - W$ model [85], where the transported variables are the turbulence kinetic energy and the square of the local frequency of the turbulent motion. Spalding immediately recognised the opportunity to use it in his EBU model, and proposed the use of W to replace the velocity gradient $|\partial u/\partial y|$ in Eq. 2. Of course, in the end it would be the kinetic energy dissipation rate ϵ that would be used, and ϵ/k would be the mixing rate used in the EBU model [57].

Spalding also stressed other aspects susceptible to refinement; among them, the fact that the mixing fluid fragments may not be just in burned and unburned states, but perhaps closer in compositional space. This is an idea that he would develop 24 years later as his Multi-Fluid Models of turbulent combustion (see below); at the time, however, he would propose the writing and solution of equations for the root mean square of the concentration fluctuation, which would become in time the second ingredient (together with the mixing frequency ϵ/k) of his EBU model.

Refined derivatives of the EBU model would appear later, such as the popular Eddy-Dissipation model (EDM) [50] and the Eddy-Dissipation Concept (EDC) [48, 49]. The EDM differs from the EBU in that it replaces the square root of the concentration fluctuations [57] in the reaction rate with the mean concentration of the deficient species (fuel for lean, or oxidiser for rich mixtures). Further, the EDM computes the reaction rate from the minimum of three rates based on the mean oxygen mass fraction, mean fuel mass fraction and the mean product mass fraction. Although the original EBU approach was developed for premixed combustion, the EDM can be used for both premixed and non-premixed combustion [50]. The EDC is an extension of the EDM that considers detailed reaction kinetics on small scales, which are modelled as a perfectly stirred constant-pressure reactor with initial conditions taken from the prevailing cell composition and temperature. The reaction rates are determined by Arrhenius expressions, and proceed over a Kolmogorov residence time.

Despite these advances from his highly influential EBU concept, Spalding regarded his Multi-Fluid Models (see below) as the heir apparent to the EBU.

3.2 The ESCIMO Model

Spalding's quest for physical fidelity in his combustion models was clearly reflected in the genesis of the EBU model as portraying the interaction of fluid parcels with different degrees of reactedness. It may be argued that, for the EBU model, the translation of such interaction into the model equations was limited by the mathematical and computational tools available at the time. Spalding would in fact often use the EBU model imagery (the colliding fluid fragments) as the basis for his successor models, while disapproving of its mathematical embodiment as inadequate.

The first significant step in the sophistication of the mathematical description was the ESCIMO model. Around 1976, Spalding contrived a means for modelling the creation of scalar isosurface by the turbulent flow. His idea was first published in a review of mathematical models of turbulent flames [89] as "the stretch-cut-superpose model of turbulent scale reduction", and is illustrated in Fig. 5.

As it was often the case in Spalding's scientific career, the spark of intuition soon developed into a new theory. He now turned his attention to the "*coherent* bodies of gas which are squeezed and stretched during their travel through the flame" [91] (the emphasis is ours). The essential ingredients of the new model were

- An equation for the time evolution of the thickness λ of a two-part layer (of the kind portrayed in Fig. 5) in a turbulent flow:

$$\frac{D\lambda}{Dt} = -\lambda R \quad , \tag{5}$$

  where R is a stretch rate, such as $R = |\partial\overline{u}/\partial y|$ in quasi-unidirectional flow.
- A probability density function for the ages $a = \exp(Rt) - 1$ of the gas parcels present at any point.
- A functional relationship, derived from the above assumptions, between the average reactedness $\overline{\tau}$ (obtained from a transport equation) and the average reaction rate $\overline{S}_\tau$.

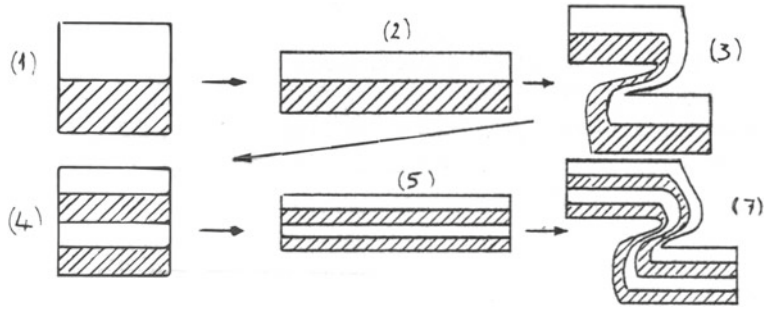

Fig. 5 The stretch-cut-superpose model of turbulent scale reduction (reproduced from [88])

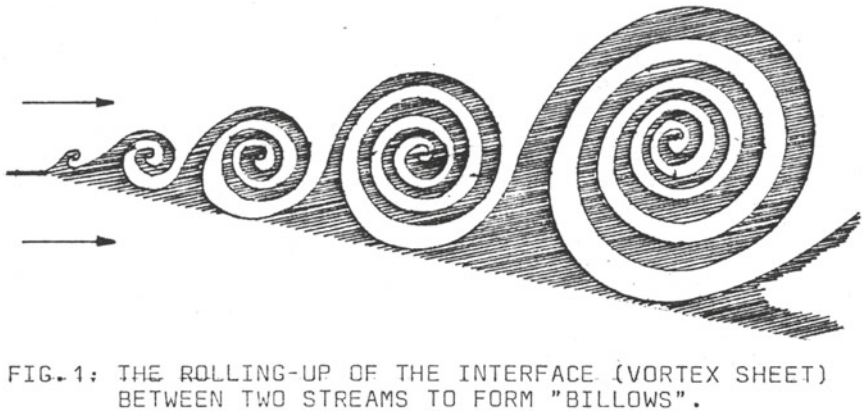

Fig. 6 Engulfment or rolling up of the iso-surface at the edge of a mixing-region (reproduced from [90])

The above ideas were soon developed into the ESCIMO model of turbulent combustion [88, 93, 110]. ESCIMO stands for Engulfment, Stretching, Coherence, Inter-diffusion, Moving Observer:

- Engulfment is the formation of layers of fluids at the mixing-region edges (Fig. 6).
- Stretching is the reduction in length scale by turbulence, for instance as mathematically described by Eq. 5.
- Coherence is the preservation of this layered structure as it moves with the flow.
- Inter-diffusion is the all-important role of molecular diffusion, enhanced by the stretching and coherence processes which increase the scalar iso-surface density.
- Moving Observer is the use of Lagrangian, parcel-attached, coordinates under which the interplay between diffusion and chemical reaction can be regarded as a one-dimensional, unsteady process.

The ESCIMO mathematical theory appears to have been formulated largely on intuitive grounds and it divides the analysis into two parts: (1) a biographic (Lagrangian) part, in which the details of reaction and molecular diffusion within folds are treated as essentially one-dimensional; and (2) a demographic (Eulerian) part, which involves the specification and description of the fold distribution. The biographic part considers what happens within the fold between its birth by engulfment, and death by re-engulfment or escape from the entire region of interest. It is here that the one-dimensional transient problem is solved including the chemical kinetics, which are assumed to obey laminar laws. The dynamics of turbulent flow are addressed in the demographic part, which "concerns the statistics of the population of coherent fluid parcels: how many of each kind are born, where they travel to, to what environmental conditions they are subjected to, and how long they live." [93].

Spalding recognised that "the components of ESCIMO are [...] familiar ones; but they [were] linked together in a special way to form a predictive method for

turbulent flames" [88]; and likened this process to the creation of new paintings from the arrangement of a finite number of colours on the canvas.

It is interesting to note that the ESCIMO model shares many features with the Linear Eddy Model (LEM) Model developed almost a decade later by Kerstein [36]. As with Spalding's ESCIMO, Kerstein's LEM also solves a differential equation for the one-dimensional diffusion-reaction process at the microscale. While in Spalding's ESCIMO the structure is convected in a Lagrangian frame, Kerstein's LEM used a cell-based, Eulerian strategy whereby fragments of the one-dimensional eddy are moved from between neighbouring cells, the size of the exchanged fragment being proportional to the convection and diffusion contributions in the discretised transport-equation coefficients. In ESCIMO, scalar gradients are increased through 'squashing' as the fluid parcel ages; in LEM, the gradients are increased by a stochastic process of artificially compressing and replicating fragments of the one-dimensional field, a process termed a 'triplet map'.

The ESCIMO model was applied to several problems, including baffle-stabilised premixed flames [46, 58], premixed well-stirred reactors [120], natural-gas diffusion flames [119] and hydrogen-air diffusion flames [14, 47, 119].

4 Two-Fluid Models

The ESCIMO model was relatively short-lived. Spalding reflected that the necessary parameters could be adjusted "to make predictions fit a limited set of experimental data", but that "time-averaged concentration profiles [...] proved hard to reproduce via ESCIMO" [97]. He attributed these difficulties to the fact that the then-prevailing turbulence model, the $k - \epsilon$ one, did not account for intermittency at the outer regions of the jet. Thus ESCIMO "emphasises the small-scale non-uniformities while leaving the large-scale ones to be handled (poorly until now) by the hydrodynamic turbulence model" [98]. He then moved on to remedy this difficulty with a new class of turbulence models: the two-phase turbulence models.

In the mid-70s, Spalding contrived a means for solving two-phase flows, with interphase slip, in an Eulerian–Eulerian framework. The so-called Inter-Phase Slip Algorithm, or IPSA [95, 113], was implemented in a number of codes. It is still nowadays one of the main algorithms for solving the Eulerian equations in multiphase flows.

In a canonic example of Spalding's ability to think unconventionally in the search for solutions, soon after developing IPSA he saw an opportunity to use the new technique to evolve a new class of turbulence models. Spalding's motivation was to address some shortcomings of conventional turbulence models, such as their inability to represent the intermittency of turbulent flow or of counter-gradient diffusion (although the latter is within the capabilities of some second-moment closures).

Conventional turbulence models employ a statistical approach [40, 71] where the unknown statistically averaged values of the turbulent fluxes of mass, heat and momentum are closed either by solving transport equations for these quantities

directly, or by using a turbulence model based on the Boussinesq [6] eddy-viscosity relationship. Most commonly used are eddy-viscosity models employing transport equations for the turbulence kinetic energy and a length scale determining variable, usually the turbulence dissipation rate [22] or turbulence frequency [40]. During the 1960s Spalding [85] pioneered the development of such models.

The new turbulence model exploited the analogy between turbulence and two-phase flow, and was called the two-fluid model of turbulence [99–101, 104, 114].

The two-fluid model is based on the notion that a turbulent fluid can be represented as a mixture of two fluids, which can be distinguished from each other in several ways, such as for example by defining the two fluids as hotter and colder, turbulent and non-turbulent, lighter and heavier, faster and slower, upward-flowing and downward-flowing, etc. Each fluid has its own temperature, composition variables, velocity components, volume fractions etc, and the two fluids interact with each other through the sharing of space and the exchange of mass, heat and momentum by the physical processes of tearing, folding, inter-diffusion and separation. The volume fractions can be regarded as 'probabilities of presence', and the interspersed fluid fragments can be characterised by one (or more) local fragment size distributions. Spalding was quick to point out that in the past "several authors have advocated thinking of a turbulent flow as a mixture of two intermingling fluids. The idea formed a part of the thinking of Reynolds [70] and Prandtl [67] as they considered how mass, momentum and energy were transported in turbulent fluids." Spalding light-heartedly likened Reynolds' intermingling-fragments concept as "stew", and Boussinesq's enlarged viscosity as "thick soup".

During the subsequent development of the two-fluid model at Imperial College it was discovered that ideas similar to those embodied in the two-fluid concept had already been proposed by several workers [11, 13, 39, 42, 117]. All of these studies were concerned with developing methods to predict intermittency within the framework of conditional zone-averaged conservation equations for the turbulent and non-turbulent zones.

4.1 Mathematical Formulation

The two-fluid turbulence model requires the simultaneous solution of two sets of differential equations which are coupled through laws defining the exchange of mass, momentum, energy and chemical species between the two fluids, which are assumed to be arranged in fragments. An additional constraint is that the volume fractions of the two fluids must sum to unity. Spalding [97, 100, 114] proposed expressions for determining the rates of exchange between the intermingling fluid fragments. These interaction terms involve the specific area of the interface between the two fluids, which Spalding proposed should be computed via a differential equation for the fragment size, with mechanisms that control its growth or diminution. In less advanced work, the fragment size is taken as proportional to some characteristic dimension of the flow.

Another important term appearing in the differential equations is the 'phase-diffusion' term, which originates from time-averaging the convection terms in the phase-continuity equations. Consequently, a related term also appears in the other differential equations where it augments the within phase diffusion term. The term is intended to represent the random-motion flux associated with the movement of the interface between the two fluids, i.e. the to-and-fro motion which occurs in addition to the mean motion of the phase in question. Spalding [99] proposed modelling this type of motion in terms of an effective diffusion coefficient and the local gradient of the volume fraction, with the former being taken as proportional to the mean rate of strain and fragment size.

4.2 Applications to Inert Turbulent Flows

Intermittent and other turbulent flows. Initial developments of the two-fluid model at Imperial College were concerned with predicting the intermittency of free turbulent shear layers. Both Malin [51–54, 116] and Xi [123], working under Spalding's direction, developed and applied two-fluid models for predicting the intermittency factor and flow variables in the turbulent and non-turbulent zones of free turbulent shear layers. These two models differed from Spalding's [99] original proposal mainly in their use of either Prandtl's mixing length [51, 54, 123] or a two-equation $k - \epsilon$ model [52–54, 116] for determining the fragment size, rather than compute it from a differential equation. Xi used a constant eddy-viscosity for modelling turbulent diffusion, whereas Malin used the eddy-viscosity computed from the turbulence model within the turbulent phase. When the $k - \epsilon$ model was used, it was modified to account for the additional production of turbulence at the interface.

Xi applied his model to steady and transient jets, both with and without buoyancy, and reported good agreement with measurements of mean and conditioned flow variables, jet-tip penetration rates, and intermittency profiles. For heated jets and wakes, Malin's model also produced results that were in reasonable agreement with both the conditioned and unconditioned data, but the intermittency factor was overpredicted for jets. This was attributed mainly to the interphase mass-transfer model not allowing for turbulent fluid to enter the non-turbulent category and so account for the physical mechanism of decay and dissipation. This deficiency was later addressed by Fan [15], who obtained much improved intermittency profiles for the round jet by adding an interphase mass sink term proportional to the mean rate of strain.

These early studies prompted Spalding [101, 104, 114, 116] to abandon the idea of classifying the two fluids as 'turbulent' and 'non-turbulent' in favour of a 'faster' and 'slower' split where turbulent fragments are presumed to be present in both fluids. The thinking was that this new approach would prove more general, because the earlier classification would be inadequate for internal flows, where downstream of the initial entrance region, there can be no non-turbulent fluid. Spalding [104] established a connection with Prandtl's mixing length theory to make three major modifications to his original two-fluid model [99]. The first was the use of a symmetric

mass-transfer law between the two fluids to allow mass transfer to take place in both directions. The second was the introduction of a shear-related source in the cross-stream momentum equations, the purpose of which was to express "the tendency of a shear layer to breakup into a succession of vortices". The third modification concerned within-phase diffusion, for which the eddy-viscosity was replaced with a diffusion coefficient proportional to the fragment size and the slip between the two fluids. This was based on the notion that the turbulent-transport properties arise from "the mixing in the wakes of the fragments in relative motion".

The revised two-fluid model was applied first by Spalding [104] to a Couette flow with heat transfer, in which the shear-induced source of cross-stream momentum drives one of the fluids upwards while the other moves downwards. Further applications were undertaken by Ilegbusi [26–28] at Imperial College under Spalding's supervision, and these culminated in joint publications [30–32] which reported satisfactory agreement with experimental data on flat-plate boundary layers and Couette flow [31], and pipe and channel flows and plane and round jets with and without heat transfer [30, 32].

All of the foregoing studies computed the fragment size from Prandtl's mixing length, but another of Spalding's students, Fueyo [18], developed the model further by computing the fragment size from a differential equation which accounted for fragment growth by entrainment and agglomeration, and fragment breakup by shear. The model was applied to the round jet and the predictions were found to be in satisfactory agreement with the experimental data. An interesting outcome of this study was that after a certain jet-development region, the centreline values of the fragment size were found to be proportional to the Prandtl mixing length.

Rayleigh–Taylor Instability. Also at Imperial College, Andrews [2] developed a two-fluid model of different density fluids for the simulation of flows involving Rayleigh–Taylor instability (RTI). Such flows are of interest in astrophysics, geophysics and nuclear fusion; and they occur whenever a heavy fluid is placed above a light one in a force field, usually gravity. The interface between the two fluids is unstable to any disturbances and becomes increasingly distorted before degenerating finally into a turbulent mixing process. Andrews [2, 4] performed a RTI experiment by overturning a stably stratified tank of two fluids, and then applied a two-fluid model of the turbulence to simulate the mixing process. This model classified the fluids as light and heavy, and a differential equation was solved for the mixing length scale with account taken of the growth and reduction in size of the fluid fragments. The results were reported to be in good agreement with the experiments.

Andrews [3] also considered the de-mixing heated-saline experiment of Stafford [118] where the RTI mixing of cold water over hot saline is followed by a de-mixing phenomenon, which occurs when there is a reversal in the pressure gradient. This is an example of a double-diffusive process where the salinity and temperature make opposing contributions to the vertical density gradient. Simulations with the two-fluid model predicted successfully both the mixing and de-mixing phenomena. Conventional turbulence models cannot address 'counter-gradient' de-mixing because the

gradient-diffusion hypothesis means that once mixing has taken place, de-mixing cannot happen.

Two-fluid descriptions of RTI have also been used by Youngs [124–127], Chen et al. [9], Llor [44, 45] and more recently by Kokkinakis et al. [38], who compared the results of a two-fluid model with those of a modified two-equation turbulence model with reference to high-resolution implicit large-eddy simulations (ILES) of compressible Rayleigh–Taylor mixing. Both the single and two-fluid models were reported to produce good agreement with ILES with respect to the self-similar mixing width; peak turbulent kinetic energy growth rate, as well as volume fraction and turbulent kinetic energy profiles. Despite being computationally more demanding, the two-fluid model was preferred because of its ability to represent the degree of molecular mixing directly by transferring mass between the two phases, and also because of its potential to model de-mixing when the acceleration reverses sign.

Metallurgical Applications. Ilegbusi [29, 33] applied the two-fluid model of turbulence to compute the flow distribution in a continuous-casting tundish, which is a broad, open bath containing molten metal with one or more holes in the bottom. These feed into an ingot mould during the casting process. Tundishes are characterised by highly turbulent flow regions near the inlet and outlet, and essentially quiescent (laminar) regions elsewhere in the bath. Consequently, the fluids were defined as turbulent and non-turbulent, and it was argued that the two-fluid concept was ideal for representing the coexisting zones of turbulent and non-turbulent flow. For both water models and steel systems, the two-fluid model produced better agreement with the measured residence times than the single-fluid $k - \epsilon$ model. The longer residence times obtained with the $k - \epsilon$ model were believed to be due to its tendency to overpredict mixing between the highly turbulent and largely quiescent regions.

Later, Sheng and Jonsson [76] and Anestis [5] employed similar two-fluid turbulence models to simulate transient flow and heat transfer in a tundish. The original liquid in the bath was defined as one fluid, and the inlet stream as the other fluid. Both studies reported that the two-fluid model showed better agreement with the measurements than the single-fluid $k - \epsilon$ model, and especially in transition and mixed-convection regions, where the two-fluid model predicted less turbulent transport. These studies confirmed Ilegbusi's [29, 33] earlier result that the two-fluid model captures the physics better when representing systems with localised highly turbulent regions and largely quiescent regions elsewhere.

Huang [24, 25], Ilegbusi [25, 34], and Pfender and Chang [65] all reported on two-fluid modelling of turbulent plasma jets, which are of interest in materials processing, including spray deposition. In all of these studies, the fluids were defined as hot (the plasma gas-argon) and cold (the ambient fluid). The results showed that the model can predict the observed unmixing and intermittency that escapes the more conventional turbulence models, which only account for gradient-diffusion mixing.

Other Applications. Shen et al. [74, 75] employed a two-fluid model based on the work of Fan [15] and Spalding [99] to simulate the turbulent stratified flow of lighter density fluid above a denser stream in a channel. This model classified

the fluids as light and heavy and the $k - \epsilon$ turbulence model was used within each phase to determine the eddy-viscosity and fragment size. The model produced good agreement with measured velocity and relative density profiles, and the collapse of the turbulence under the influence of strong stable stratification was predicted correctly.

Yu et al. [128] applied two-fluid turbulence modelling to simulate the flow and heat transfer characteristics of air curtains in an open refrigerated display cabinet. The asymmetric and symmetric forms of the mass-transfer rate were investigated, as well as a weighted mean of the two relations. The fluids were classified as turbulent (the air curtains) and non-turbulent (the ambient air outside the cabinet), and the $k - \epsilon$ model was used within the turbulent phase. The two-fluid model was found to give better agreement with the measurements than the single-fluid $k - \epsilon$ model, and so a better prediction of the air curtain, the thermal field outside the case, and the cold-air overspill from the case into the store. This same two-fluid model was used later by Cao et al. [8] in combination with machine-learning methods to produce a strategy for optimising the design of air curtains for open-display cabinets.

Liu et al. [43] applied the revised two-fluid model of Spalding for predicting the turbulent flow in a closed-conduit polychromatic UV disinfection reactor. These types of reactors are widely used in treating both drinking water and wastewater. In addition to the turbulence modelling, this challenging application also included a fluence-rate model for the UV light-intensity distribution, and a microbial inactivation kinetic model to represent the fluence response of target microorganisms. In the two-fluid model, the fragment size was computed from the differential equation of Fueyo [18]. Overall, the results compared reasonably well with the measurements, but no better than those produced by four other single-fluid two-equation turbulence models and a second-moment closure.

More recently, Zhang et al. [129] used Spalding's two-fluid concept to develop a turbulence model based on the EMMS (energy-minimization multi-scale) method [41] for fluid-solid systems. This EMMS-based turbulence model regards single-phase flow as a mixture of turbulent and non-turbulent fluids; and a multi-scale analysis divides the energy of the turbulence into three separate scales: a molecular scale, an eddy scale and a macro scale. A turbulence stability condition plus several constraint equations are then used to close a set of turbulent dynamic equations, which are then solved to produce optimised values of the volume fraction and diameter (fragment size) of the turbulent eddies. For any given flow system, using as input the superficial velocity of the turbulent eddies and some other parameters, the volume fraction and fragment size are computed in advance of the CFD simulation. The EMMS-based turbulence model then uses a table in the CFD simulation to modify the local values of the eddy-viscosity produced by a conventional turbulence model. This novel approach was applied to simulate lid-driven cavity flow and turbulent forced convection in an empty room. The EMMS-based models showed improved performance over the unmodified turbulence models by capturing the detailed secondary and tertiary vortices in the corners of both the cavity and the room. It was argued that the standard models were less successful because they regard the fluid to be in a turbulent state everywhere, but near walls and especially in the corners,

viscosity dominates rather than inertia, and so the fluid should be close to laminar instead of fully turbulent. In contrast, the EMMS-based turbulence model treats the flow everywhere as a mixture of laminar and turbulent fluids.

4.3 Applications to Combustion

Spalding's inspiration for the development of two-fluid models of turbulence was perhaps the fragmentariness exhibited by many classes of turbulent flow. Such fragmentariness is seldom more apparent than in a turbulent flame, where burned and unburned fragments intermingle at the flame front. To describe graphically the model concept, Spalding used the image of a rugged coastline, "with many islands and land-locked lagoons" [100] as shown in Fig. 7. (For historical interest, the figure also shows one Spalding's hallmark lecture panels. In a private conversation in 2008 with one of the present authors, NF, Spalding humorously shared his belief that such format was possibly his greatest contribution to Science.)

Internal combustion engines were perhaps the inspiration for Spalding's Two-Fluid Models, possibly because they exhibit, like no other flow, "patchiness": sharp changes in fluid properties (temperature, composition, perhaps even velocity) over small distances [98].

Combustion Two-Fluid Models are described by the averaged multiphase Eulerian equations. For a generic variable ϕ_i in phase i (such as momentum per unit mass,

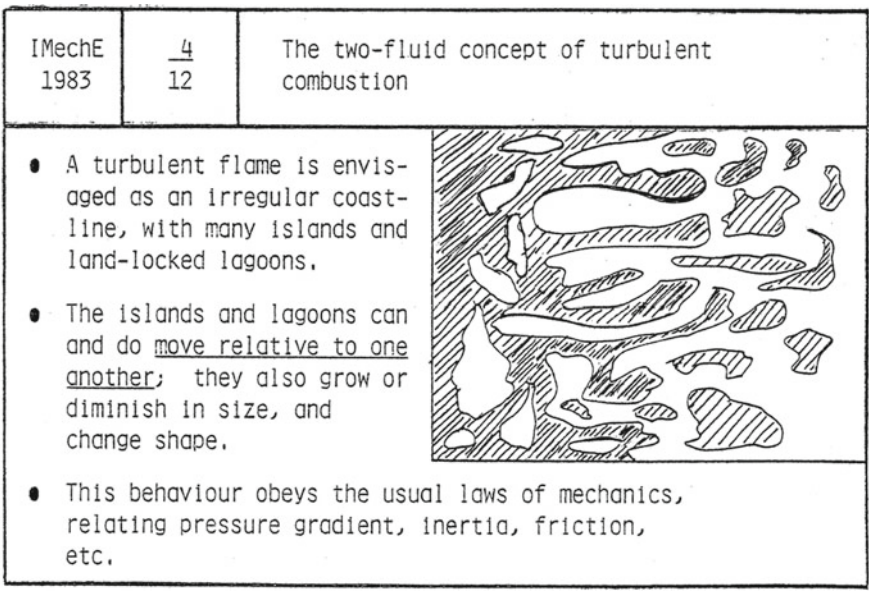

Fig. 7 Spalding's lecture panel, portraying a flame front as an irregular coastline, with islands and land-locked lagoons. Reproduced from [100]

mass fraction, enthalpy per unit mass), its transport equation is (the overbar denoting averaging being dropped for simplicity)

$$\frac{\partial\left(\rho_i r_i \phi_i\right)}{\partial t} + \nabla\cdot\left(\rho_i r_i \phi \mathbf{v}_i\right) - \nabla\cdot\left(\Gamma_r \phi_i \nabla r_i\right) - \nabla\cdot\left(\Gamma_\phi r_i \nabla\phi_i\right) = S_{\phi_i} + f_{ji}\left(\phi_j - \phi_i\right) + [[\dot{m}_{ji}]]\phi_j - [[-\dot{m}_{ji}]]\phi_i \quad , \tag{6}$$

where

- r_i is the volume fraction of phase i.
- Γ_ϕ is a diffusion coefficient, encompassing turbulent diffusion if an eddy-viscosity model is used.
- S_{ϕ_i} is a source term, such as a component of the pressure gradient in the momentum equation.
- f_{ji} is an interphase diffusion coefficient (such as drag, or heat transfer between the phases by combustion).
- $\dot{m}_{ji}$ is the interphase mass-transfer rate from phase j into phase i.
- $[[\odot]]$ indicates the maximum of 0 and $\odot$.

The equation for the volume fraction r_i of fluid i is

$$\frac{\partial\left(\rho_i r_i\right)}{\partial t} + \nabla\cdot\left(\rho_i r_i \mathbf{v}_i\right) - \nabla\cdot\left(\Gamma_r \nabla r_i\right) = \dot{m}_{ji} \quad . \tag{7}$$

The mass-transfer rate between the fluids $\dot{m}_{ji}$ is a crucial parameter in Two-Fluid Models. It accounts for the entrainment of one fluid into the other. Several formulations were proposed at the time, usually involving a relative phase velocity, $\left|\mathbf{v}_i - \mathbf{v}_j\right|$ and a fragment size l (or equivalently the interface surface area per unit volume l^{-1}), for which a model needs to be provided.

Spalding [102] discusses the potential of the two-fluid model for simulating a wide range of combustion problems, but practical applications appear to have been limited to transient one-dimensional premixed flames [55, 102, 122] and unbounded fire plumes [56].

Spalding regarded [106] his earlier Eddy Breakup Model as a precursor to his Two-Fluid Model, in which the two fluids were the fresh reactants and the burned products. He also viewed the Eddy-Dissipation Concept of Magnussen [49], flamelet models of combustion [63], and the Bray–Libby–Moss model [7] as two-fluid models embodied in single-phase frameworks.

4.4 Concluding Remarks

Spalding's Two-Fluid Model was a novel approach for modelling turbulence that provided an alternative formulation capable of predicting intermittency and counter-gradient diffusion. Also, unlike any single-fluid turbulence model, the model can

portray adequately the interactions of pressure gradients and density fluctuations which are major sources of generation of turbulent motion in certain applications. Despite these advantages the model failed to gain widespread popularity because it offered no superiority over conventional models for most engineering and environmental applications. For general usage, the two-fluid concept was hard to grasp because of uncertainty over the best characteristic to use for distinguishing the two fluids. Another deterrent was the increased computer time and convergence demands associated with the need to solve twice as many differential equations, as compared to conventional models.

Spalding later concluded that in one respect, the Two-Fluid Model was over-elaborate on the grounds that the relative velocities of the fluids are often small enough to be neglected, or computed by way of an algebraic-slip approximation, which permits extension to the treatment of the relative motion of more than two fluids, which is what is needed for greater realism. This led Spalding to turn his attention to multi-fluid turbulence models.

5 Population-Type Multi-fluid Models

In the mid-90s, Spalding concluded that two fluids did not suffice to represent the complexity of the composition field in combustion situations, and adopted the idea of Multi-Fluid Models of turbulent combustion. Unlike Two-Fluid Models, which were multiphase in nature, Spalding's Multi-Fluid Models are single-phase, and based on the idea of discretising one or several relevant fluid properties. The notion of discretising properties was not new to Spalding. The six-flux model of radiation discretised the radiation fluxes in positive and negative directions [94], and non-slip clouds of particles had been discretised into particle sizes.

At the time, Spalding was aware of the particle-based Monte Carlo methods for solving the multi-dimensional composition Probability Density Function (PDF) in turbulent combustion [66], and often saw the newly born Multi-Fluid models as a more economical way to compute the PDF [79]. Striving as always to find the best word to describe an idea, he often referred to these Multi-Fluid Models as "Population Models", in that the fluid is represented by an ensemble of fluids, each fluid in the ensemble being a population member.

5.1 A Four-Fluid Model

The inspiration for Multi-Fluid Models appears to have presented itself to Spalding around 1995 [115] as he reflected on the limitations of his popular Eddy-Breakup Model, and its widely adopted successor the Eddy-Dissipation Model of Magnussen.

The Eddy-Breakup Model, under the Multi-Fluid lens, consisted of just two "fluids": one is the fresh mixture of fuel and oxidant, and other is the completely burned

products of their combustion. Of course, intermediate states of partially burned mixture do exist in the flame, but they were assumed to be confined to very thin layers in the interface between both, and hence were neglected in the overall thermodynamics of the mixture. Flamelet models [64] place special importance on this interface region. Spalding would at some point draw a similarity between flamelet models and his Multi-Fluid ones [78], the nexus being the notion of an 'encounter' between fluid parcels whereby they "approach and make contact; remain in contact for a short time, say T_{cont}; and then separate". This process, and the contact time, is the essence of his Multi-Fluid Models.

The first stepping-stone in the development of a Multi-Fluid Model was a Four-Fluid Model. The model was originally contrived as a means of obtaining greater realism than the original Eddy-Breakup Model could afford. While the original Eddy-Breakup Model consisted only of fresh, unburned reactants (R) and fully burned products (P), the new Four-Fluid Model allowed for two mixtures of these: a non-reacting mixture (N) of reactants and products (with given, fixed proportions) that is too cold to burn, and a mixture (K) of reactants and products (with given, fixed proportions) that can burn (their burning rate being controlled by chemical kinetics). Therefore, unlike the single pathway from R to P in the original Eddy-Breakup Model, the new model allowed for three parallel routes:

$$\mathrm{R} + \mathrm{P} \rightarrow \mathrm{K} \rightarrow \mathrm{P} \tag{8}$$

$$\mathrm{R} + \mathrm{P} \rightarrow \mathrm{N}; \mathrm{N} + \mathrm{P} \rightarrow \mathrm{K} \rightarrow \mathrm{P} \tag{9}$$

$$\mathrm{R} + \mathrm{K} \rightarrow \mathrm{N}; \mathrm{N} + \mathrm{P} \rightarrow \mathrm{K} \rightarrow \mathrm{P} \tag{10}$$

Thus, while the original Eddy-Breakup Model consisted only for states R and P, the Four-Fluid Model allows for intermediate states N and K; and, crucially, both mixing and chemical reaction have an influence on the overall rate of conversion, as will be discussed next.

The last reaction in all the pathways is the creation of newly burned products P from flammable mixture K; such creation was controlled by chemical kinetics, thus allowing "chemical-kinetic effects to be introduced rationally" in the model:

$$\dot{m}_{\mathrm{P}} = m_{\mathrm{K}} R_{\text{chem}} \quad , \tag{11}$$

where R_{chem} is a kinetic rate (e.g., given by an Arrhenius law).

The remaining steps are mixing-controlled, and are modelled, similar to the Eddy-Breakup Model, using the turbulence kinetic energy k and its rate of dissipation ϵ; for instance, for the first reaction, the rate of creation of mass of K fluid would be

$$\dot{m}_K = C m_R m_P R_{\text{mix}} \quad , \tag{12}$$

and the corresponding sinks for R and P. Here, C is a constant that may vary for each reaction step.

The mixing rate R_{mix} may be given by a mechanical mixing rate, such as (in the original Eddy-Breakup model):

$$R_{\text{mix}} = \frac{\epsilon}{k} \quad . \tag{13}$$

The Four-Fluid Model was demonstrated by Spalding in simple geometries. The first one was, incidentally, "the same problem as that for which the EBU was invented, namely, that of steady turbulent flame spread in a plane-walled duct". He reported [80] that his new Four-Fluid Model exhibited a similar qualitative behaviour as in the experiments of [121] *viz* that the rate of spread of the flame very little depends on the fuel-air ratio, the velocity or the temperature of the incoming mixture.

A transient version of the Four-Fluid Model was also used to predict flame propagation in a duct with baffles [16], and an explosion in an off-shore platform [17].

More recently, Hampp and Lindstedt [21] have used the multi-fluid concept of Spalding to identify, experimentally, burning regimes at low Damköhler numbers. Hampp and Lindstedt employ simultaneous Mie scattering, PIV and OH-PLIF to identify, in the flame, fluid fragments in one of the following categories: fresh reactant fluid, mixing fluid, mildly reacting fluid, strongly reacting fluid and product. This classification is very similar to that employed by Spalding in the four-fluid model just described; Hampp and Lindstedt, however, use two categories to represent the reacting fluid.

5.2 Population Models

Spalding soon concluded that the main benefit of the foregoing Four-Fluid Model would be educational [106] (because of its simplicity and economy), and that more realism would require more fluids. The generalisation was in the form of population models, where the flow is made up of a number of 'fluids'. The key ideas in Multi-Fluid Models are

1. Fluids are distinguished from one another through one or several properties (such as mixture fraction, or the concentration of a chemical species, or temperature) called Population-Distinguishing Attributes.
2. The value of such a property in a fluid is constant, and different from that in other fluids, so that all the fluids combined *discretise* the property.
3. Fluid parcels coalesce and mix, exchanging mass and properties and creating intermediate, or "offspring", fluids.
4. Further, the increase in the value of the property in the flow is represented by mass transfer from fluids with low values to fluids with high values (and conversely for the decrease); this process is referred to below as *transport in population space*.
5. The fluids also have non-discretised properties, called Continuously Varying Attributes. These are also exchanged as the fluids coalesce and mix.

5.2.1 The Population-Distinguishing Attributes

In Multi-Fluid Models, the properties that are used to distinguish each fluid are called Population-Distinguishing Attributes, or PDAs. In a non-premixed flame, for instance, mixture fraction is a prime candidate for a PDA: the mixture-fraction space will be discretised, and different fluids will have different (but fixed) values for the mixture fraction; this is a one-dimensional fluid population. Additional properties may be needed for other problem classes. For instance, a reaction-progress variable, such as reactedness, may be additionally required, resulting in a two-dimensional fluid population.

Figure 8 represents a one-dimensional fluid population where the population-distinguishing attribute is a generic variable ξ. This is discretised into 'bins', each with a constant value of the variable ξ; for fluid γ, this value is ξ_γ, and m_γ is the mass fraction of the overall fluid with this value of ξ.

For the mass fraction of fluid γ, m_γ, a conservation equation is solved

$$\frac{\partial(\rho m_\gamma)}{\partial t} + \nabla \cdot (\rho \mathbf{v} m_\gamma) - \nabla \cdot (\Gamma_\gamma \nabla m_\gamma) = \dot{m}_\gamma \quad . \tag{14}$$

To be clear, this is not the conservation equation for the mass fraction of a species γ, as in a conventional turbulence model; it may be, in a Multi-Fluid Model, the mass fraction of fluid γ with a given fixed value, for the mass fraction of a chemical species. The terms on the left-hand side of the equation are the usual transient, convection, and diffusion terms in the Eulerian conservation equation, representing accumulation and transport in physical space. The local velocity $\mathbf{v}$ is often presumed to be the same for all the fluids, albeit Spalding envisaged ways to remove this limitation, for instance, if the density of the several fluids differ so much as to make their different response to body forces relevant; also, the diffusion coefficient Γ_γ is taken as being the same for all fluids.

The source term in Eq. 14 accounts for two distinct processes in the context of Multi-Fluid Models: the exchange of matter between fluids as they collide and mix, $\dot{m}_\gamma^{\text{mixing}}$, and transport in population space (for instance, in *compositional* space due

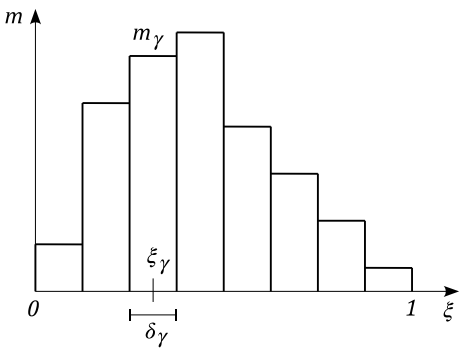

Fig. 8 A one-dimensional fluid population using a generic distinguishing attribute ξ, arbitrarily varying between 0 and 1

to chemical reaction if the attribute γ is composition-related), $\dot{m}_\gamma^{\text{convection}}$:

$$\dot{m}_\gamma = \dot{m}_\gamma^{\text{mixing}} + \dot{m}_\gamma^{\text{convection}} \quad . \tag{15}$$

These are explained in the next subsections.

5.2.2 Fluid-Fragment Collision and Mass Exchange

The notion of fluid-fragment collision and mass exchange is central to Spalding's Multi-Fluid Models; it is often referred to by Spalding as "coupling and splitting", and is akin to the concept of micro-mixing, or molecular mixing, used in transported-PDF combustion models [69]. The physical image of 'Spalding's micro-mixing' is that fragments of two fluids briefly collide, partially mix, and then separate leaving some "offspring". In his own words [108]:

1. "Two fragments of fluid are brought into temporary contact by the random turbulent motion [...];
2. Molecular and smaller scale turbulent mixing processes cause intermingling to occur [between] the coupling fragments;
3. Before the intermingling is complete, however, the larger scale random motions cause the fragments to be plucked away again, with the result that the amounts of the material having the compositions of the parent fluids [...] are diminished, while some fluid material of intermediate composition has been created [...]."

The rate of micro-mixing can be computed in several ways. A general model proposed by Spalding is

$$\dot{m}_\gamma^{\text{mixing}} = \sum_{\alpha,\beta} \rho F_{\alpha\beta}^\gamma m_\alpha m_\beta T_{\alpha\beta} \quad . \tag{16}$$

In this equation, $F_{\alpha\beta}^\gamma$ is the fraction of fluid from the encounter between fluids α and β that enters fluid γ; and $T_{\alpha\beta}$ is a turbulence frequency (with dimensions s^{-1}).

Spalding stated [108] that "the crux of multi-fluid modelling lies in the formulae chosen for [these] functions", and that "physical intuition, mathematical analysis, guess-work and computational parsimony all play a part in their choices".

He nevertheless suggested a simple, intuition-based equation for $F_{\alpha\beta}^\gamma$:

$$F_{\alpha\beta}^\gamma = \begin{cases} -0.5 & \text{if } (\gamma = \alpha \text{ or} \gamma = \beta) \text{ and } (\beta > \alpha + 1) \\ 0 & \text{if } \gamma < \alpha \text{ or } \gamma > \beta \text{ or } \beta = \alpha + 1 \\ \frac{1}{\beta - \alpha - 1} & \text{otherwise} \quad . \end{cases} \tag{17}$$

For the mixing frequency $T_{\alpha\beta}$, he suggested that it should be independent of the parent fluids. His most often-used proposal, connecting with the origins of the Eddy-

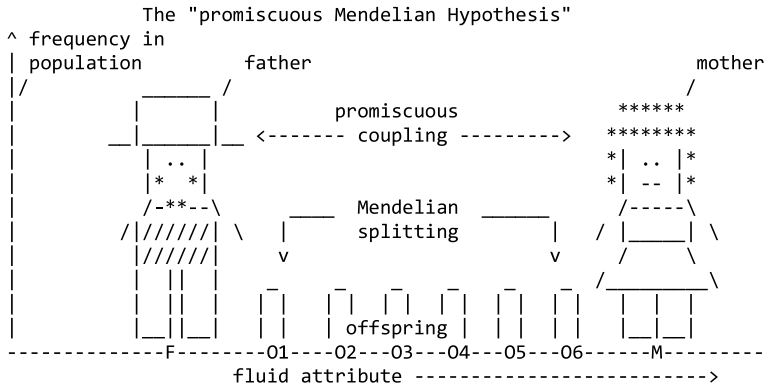

Fig. 9 The "promiscuous-Mendelian" mixing model as illustrated by Spalding [108] using ASCII art

Breakup Model and its successors, is to use a kinetic-energy decay-frequency, such as ϵ/k if the $k-\epsilon$ turbulence model is used.

Which parent fluids α and β collide and the nature of the offspring γ are key aspects of Spalding's micro-mixing models. He termed the above-described model as "promiscuous-Mendelian". The model was often illustrated by Spalding using the ASCII art rendition shown in Fig. 9 [108]. The promiscuity attribute is given because any two parent fluids α and β may collide; the Mendelian aspect is due to the offspring fluids γ possessing, in varying proportions, the attributes of either parent.

5.2.3 Transport in Population Space

When a flow property (such as temperature, or mixture fraction) is a PDA, the property is discretised and given a *constant* value from this discretisation in each of the fluids making up the population (see Fig. 8). For instance, if a PDA is temperature then the fluid is regarded as made up of N component fluids having different temperature levels $T_1 < T_2 < \cdots < T_N$.

This bears the question of how the flow property, e.g. temperature, increases or decreases its value at a point in the domain as a consequence of property sources and sinks (for instance, changes in temperature in the flow through heating). Fluid-fragment collision (or "coupling and splitting", or micro-mixing), discussed above, changes the amount mass in the involved fluids, but not the value of the property as a whole in the flow, since there is no net gain or loss of property in the exchange brought about by the collision.

Therefore, in Multi-Fluid Models, sources or sinks of a property are implemented by shifting the fluid population distribution towards higher or lower values of the property, via fluid-to-fluid mass transfer.

Let us assume that, for a fluid γ, a PDA ξ has a value ξ_γ (constant); that the mass fraction of fluid with such value for ξ is m_γ; and that the property ξ is changing locally in the flow at a rate $\dot{\xi}$ (see Fig. 8); then, Spalding [108] indicates that the mass source of fluid γ is

$$\dot{m}_\gamma^{\text{convection}} = \begin{cases} \dot{\xi}\rho\frac{m_{\gamma-1}}{\delta_{\gamma-1}} & (\text{from fluid}\,\gamma-1\,\text{to fluid}\,\gamma)\,\text{if}\,\dot{\xi}>0 \\ \dot{\xi}\rho\frac{m_{\gamma+1}}{\delta_{\gamma+1}} & (\text{from fluid}\,\gamma+1\,\text{to fluid}\,\gamma)\,\text{if}\,\dot{\xi}<0 \end{cases} . \tag{18}$$

Here, δ_γ is the width of the γ interval in PDA space, see Fig. 8. Opposite sinks must be provided for the donor fluid, so that mass is preserved.

5.2.4 Continuously Varying Attributes

PDA's have discrete values, each represented by a fluid. In addition, the fluids may have non-discretised properties, which Spalding termed Continuously Varying Attributes, or CVA's. For instance, in a turbulent combusting flow one may choose the mixture fraction as a PDA, and hence have a number of fluids each with a set value for the mixture fraction; then, each fluid may have a continuously varying value of (for instance) nitrogen-oxide mass fraction.

The transport equation for a continuously varying property ϕ_γ in fluid γ (the local mass fraction of which is m_γ) is

$$\frac{\partial\left(\rho m_\gamma \phi_\gamma\right)}{\partial t} + \nabla\cdot\left(\rho \mathbf{v} m_\gamma \phi_\gamma\right) - \nabla\cdot\left(\Gamma_\gamma \nabla m_\gamma \phi_\gamma\right) = S_{\phi_\gamma} . \tag{19}$$

The last term on the left-hand side represents diffusion processes, and the term on the right-hand side is the source of ϕ_γ. Such source will usually encompass three distinct contributions.

The first one is the within-fluid source, due, for instance, to chemical reaction (if the CVA ϕ_γ is chemical species) or to heat transfer by radiation (if the CVA ϕ_γ is temperature or enthalpy).

The second contribution to the source term, say $S_{\phi_\gamma}^{\text{mixing}}$, is the contribution from the coupling and splitting process. In the simplest model, when fragments of (say) fluid α and β collide to create fluid γ, the source of ϕ_γ due to mixing is taken as the average of the parents' values:

$$S_{\phi_\gamma}^{\text{mixing}} = \dot{m}_\gamma^{\alpha\beta}\frac{\phi_\alpha+\phi_\beta}{2} . \tag{20}$$

(Readers familiar with transported-PDF methods will recognise the similarity with the Linear Mean Square Estimation, or LMSE, model of Dopazo [10].)

The third contribution is an 'inter-fluid' diffusion of the CVA; for instance, if the CVA is enthalpy, the heat exchange due to fragment-to-fragment heat transfer between two fluids.

For both PDA's and CVA's, the local mean of the property can be computed from the fluid population distribution; for instance, the local average of CVA ϕ is

$$\overline{\phi} = \sum_{\gamma} m_{\gamma} \phi_{\gamma} \quad . \tag{21}$$

Other moments can be computed similarly.

5.3 *Towards Population CFD*

In the Four-Fluid Model presented in Sect. 5.1, the fluids were distinguished by their reactedness. Spalding's next step towards 'population CFD' was to increase not only the number of fluids, but also the number of attributes used to distinguish the fluid population.

In this Fourteen-Fluid Model [105], the compositional space is discretised along the reacted fuel fraction *and* the mixture-fraction dimensions, as indicated in Fig. 10. (The reacted fuel fraction measures reaction progress, and is akin to reactedness.) Thus fluids 1 and 14 are the original fluid streams (say air and fuel, respectively); fluids 13–16 are those with stoichiometric composition, and a varying progress of reaction. Dashed fluids in Fig. 10 are not compositionally accessible (because the reacted fuel fraction cannot exceed the mixture fraction), and thus even if the underlying discretisation of the compositional space is 5×4, only fourteen fluids are used.

Thus,

- "Fluids 6, 11, 16 and 20 are supposed to contain no unburned fuel; they thus represent completely burned gases, of various fuel-air ratios, which can react no further.

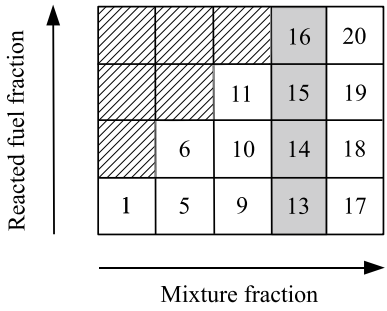

Fig. 10 Fluid population in the Fourteen-Fluid Model

- Fluids 5, 9, 13, 14, 17 and 18 contain finite amounts of free fuel; but they are regarded as being too cold to burn, like fluid [N] above.
- Fluids 10, 15 and 19 both contain fuel and are hot enough to burn; it is therefore they which, like fluid [K] in the four-fluid model, carry out the chemical reaction process. Fluid 10 thus becomes transformed into 11, fluid 15 into 16, and fluid 19 into 20."

This Fourteen-Fluid Model was applied by Spalding to the simulation of a Bunsen burner-type flame [105].

Spalding also exemplified the use of models with large numbers of fluids [108], albeit for 0-dimensional (in space) problems. Thus, he used a 100-fluid model to solve a "well-stirred reactor" (a partially stirred reactor is a more common name), where unreacted and fully reacted mixtures entered, and a partially reacted mixture exited). Since there is a single mixture fraction, a one-dimensional population suffices, with reaction progress (or reactedness) as the distinguishing attribute.

He also demonstrated a similar calculation of a non-premixed reactor, where fuel and oxidant enter separately, mix and burn. In this case, a two-dimensional population of fluids is required, with mixture fraction and reactedness as population-distinguishing attributes. He used increasingly large 'population grids' of 3×3, 5×5, 7×7 and 11×11 fluids, showing that the last two where accurate enough.

Practical applications of Multi-Fluid Models to turbulent diffusion flames have been reported by Zhubrin [130].

Around 2010, Spalding started using the concepts of "populational modelling" and even "populational CFD" [109] to describe this new type of model that, he thought, would revolutionise CFD. Indeed, Spalding last ideas on the subject were published posthumously with the appellation "The Discretised Population Model of Turbulence" [77].

6 Conclusions

Spalding's nearly 70-year scientific career is heaving with ground-breaking contributions; a large fraction of them were in the field of combustion.

His underlying vision of turbulent combustion was that of fragments of fluids with different compositions and temperatures colliding and mixing, thus creating opportunities for chemical reaction to take place.

This was indeed the *leit-motiv* of his Eddy-Breakup Model. The limited tools available at the time resulted in its embodiment in a simple mathematical expression that, although widely used due to its simplicity and much refined in subsequent evolutions, was clearly seen by Spalding as constraining.

A first attempt at removing the constraints was the ESCIMO model. Although it did enjoy some success, it was short-lived. The ESCIMO model is similar in concept to Kerstein's Linear Eddy Model.

From the early 1980s, and thanks to the emergence and widespread use of two-phase Eulerian–Eulerian models, Spalding turned his attention to their use for the modelling of turbulent flows in general, and of turbulent combustion in particular. For these, these multiphase models had the advantage of allowing for locally high density differences, and thus for accounting for the effect of body forces in turbulent combustion, such as counter-gradient diffusion.

Multiphase two-fluid models quickly evolved in the 1990s into single-phase, multi-fluid models. Spalding viewed these models as an alternative to transported-PDF models, and used the term "populational CFD" to refer to extensions of his theory to other fields, including turbulent non-reacting flows. He would dedicate to his multi-fluid models, or populational CFD, a great fraction of the latter part of his career; they often featured in his talks and presentations as he continued to travel the world to share, with undiminished stamina, his vision of combustion, CFD and Science.

Annex: A Rough Chronology

See Table 1.

Table 1 A rough timeline of Spalding's career in Combustion. Dates are approximate

DBS	Others	Milestone
1951		Ph.D. Thesis, Pembroke College, University of Cambridge
	1953	First numerical computations of combustion [23]
1954		First numerical computations "by graphical means"
1955		Textbook'Some Fundamentals of Combustion', Butterworth Scientific
1955		Analogue combustion model
1961		First numerical calculations
1968		First CFD calculation of recirculating flows with combustion
1969		GENMIX
1970		Presumed-PDF modelling of turbulent diffusion flames
1971		Numerical prediction of laminar flame propagation
1971		Eddy Breakup Model
	1972	First 3D simulation of a combustion chamber
1973		First 3D combustion simulation
	1974	Transport equation for the PDF [12]
1976		ESCIMO
	1977	Eddy Dissipation Model
	1977	BML model
1980		IPSA: Eulerian, multiphase algorithm
	1981	First Monte Carlo method for solving the transport eq. for the PDF [66]
	1981	Eddy Dissipation Concept
1982		Two-Fluid Models of turbulence
	1984	Computational implementation of flamelet models by Peters [63]
1995		Multi-Fluid Models of combustion

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