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# A tribute to D.B. Spalding and his contributions in science and engineering

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ABSTRACT

This paper presents a summary of some of the scientific and engineering contributions of Prof. D.B. Spalding up to the present time. Starting from early work on combustion, and his unique work in mass transfer theory, Spalding's unpublished "unified theory" is described briefly. Subsequent to this, developments in algorithms by the Imperial College group led to the birth of modern computational fluid dynamics, including the well-known SIMPLE algorithm. Developments in combustion, multi-phase flow and turbulence modelling are also described. Finally, a number of academic and industrial applications of computational fluid dynamics and heat transfer applications considered in subsequent years are mentioned.


## 1. Introduction

In May 2008, an International Symposium (CHT'08: Advances in Computational Heat Transfer) was held in Marrakech, Morocco under the auspices of the International Centre for Heat and Mass Transfer in honour of Prof. Brian Spalding's 85th birthday. The conference included a keynote lecture by Prof. Spalding himself and some lectures describing his research contributions. At the conference, it was decided that a special issue of this journal would be published in Prof. Spalding's honour. Whereas this issue will have invited papers on a variety of topics, it seemed appropriate to include also an extensive review of Spalding's research contributions. With this thought, the authors of this paper (most of whom have closely worked with Prof. Spalding) had a meeting at the conference to plan the nature and the structure of this paper. The discussion at that meeting and several months of work thereafter have culminated in this tribute.

Here, the authors have not just given a factual summary of Spalding's publications. They have tried to take the reader on a historical journey to show the development of his key ideas and their subsequent impact. The authors have shown how the theme of generalization or unification runs through all his work. It is this grand vision that enabled Spalding to make so many break-through contributions. In this paper, the reader will get an insight into this great man's way of thinking and his extraordinary impact on science and engineering. The authors have all greatly enjoyed the activity of writing this paper and, in the process, re-lived the experience of working with Prof. Spalding.

## 2. Nomenclature

In a paper of this nature, the usual Nomenclature section is not required. Spalding's passions for science and poetry are well

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[1] Eddie Leonardi passed away on 14 December 2008.

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known. It is perhaps the interplay between these seemingly disparate pursuits that has given him the talent to invent wonderfully descriptive acronyms that describe many of his scientific contributions. The list is long; only a few are provided here.

| | |
|---|---|
| PHOENICS | Parabolic, Hyperbolic Or Elliptic Numerical Integration Code Series |
| CHAM | Originally Combustion, Heat and Momentum Ltd.; later (since 1974) Concentration, Heat and Momentum Ltd. |
| CORA | COmbustion and Radiation Analyser |
| ESCIMO | Engulfment, Stretching, Coherence, Inter-diffusion, and Moving Observer |
| FLASH | FLow Around Ships' Hulls |
| FLIRT | FLow In Right angled Tee junctions |
| IPSA | InterPhase Slip Algorithm[a] |
| MOSIE | Movement Of Smoke In Enclosures |
| PICALO | PIston and Cylinder CALculatOr |
| SIMPLE | Semi-Implicit Method for Pressure-Linked Equations |
| THIRBLE | Transfer of Heat In Rivers, Bays, Lakes and Estuaries |

[a] Sometimes also referred to as InterPhase Slip Analyser.

Others are sprinkled throughout this paper.

## 3. Early work

The origins of Spalding's life-long contributions to heat and mass transfer and to combustion go back to his Ph.D. Thesis at Cambridge University [1]. This thesis introduced the elements that were later to govern his professional career. His goal was to understand the combustion of liquid fuels. Spalding came to the conclusion that aerodynamic flow, heat transfer and mass transfer all play key roles in a synergistic manner. To understand these phenomena, Spalding then used key hydrodynamic concepts from von Kármán [2], heat transfer concepts from Kruzhilin [3], and mass transfer concepts from Eckert and Lieblein [4]. Of course the interaction of chemical kinetics and flow processes plays a key role in combustion. Spalding also benefited from the work of Zeldovich and Frank-Kamenetskii [5,6], and of Semenov [7].

Subsequently, he went on to make the then unforeseen prediction that the chemical-reaction-rate constants had no influence on combustion until a critical rate of mass transfer was reached. He deduced these critical rates from his theory that were borne out by experiments. He also developed a methodology to predict flame extinction from this theory. This work was later expanded and published in book form, Spalding [8].

Until the early 1960s Spalding continued to work on combustion and burning of droplets and made a number of innovative contributions. These included the concept of the mass transfer driving force $B$, defined below, also known as the Spalding number. These efforts culminated in his remarkable book on convective heat and mass transfer [9]. Moreover, during this time, he also expanded his efforts to include general engineering flows in which wall shear plays an important role. This would lead to his outstanding insights and the proposal of what came to be known as "The Unified Theory". Prior to the development of finite-volume schemes, solutions to problems in convective heat and mass transfer involved the replacement of diffusion terms with rate equations, based on the notion of a heat/mass transfer coefficient, which Spalding denoted by $g$. The ability to obtain mathematical solutions to the resulting ordinary differential equations was thus central to the science of heat and mass transfer. Spalding's major contribution to mass transfer was to unify (generalize) the problem, so that essentially the same systematic approach could be applied across a range of disciplines from cooling towers to ablation to combustion. Previously, and within the separate disciplines of either heat, mass or momentum transfer, varying approaches had been used to formulate the governing equations. As a result he showed that generalized transport equations could be applied to essentially all the state-variables in fluid mechanics and heat/mass transfer, and indeed to 'synthesized' variables such as mixture fraction. This generalization of the equations of motion was pre-requisite to the subsequent development of generalized solution methodologies to engineering mechanics problems. Spalding's mass transfer formulation was firmly based on mass fractions, as opposed to molar-based balances, it being reasoned that mass (not moles) was conserved in chemical reactions, and moreover mass-weighted mixture velocities are typically obtained in solutions of the Navier–Stokes equations. Indeed, the general form of the transport equation he derived became the natural equation into which all others were forced and extra terms that did not fit into the substantive derivative, diffusion, production or dissipation terms were lumped as sources (or sinks).

In 1960, Spalding published a pioneering article [10] in vol. 1 of this journal, in which he postulated the 'Ohm's law' of mass transfer, namely

$$\dot{m}'' = gB \tag{1}$$

where $\dot{m}''$ is the mass flow ('current'), $g$ is a 'conductance' or mass transfer coefficient which depends only on aerodynamic and not thermodynamic factors, and $B$ is a mass-transfer driving force (potential) given by $B = (P_G - P_S)/(P_S - P_T)$. $P_G$ and $P_S$ are the values of some conserved quantity, $P$, in the bulk and at the wall surface of the fluid, respectively, and $P_T$ represents the 'transferred substance state' or 'T-state'. In later years the symbol '$P$' was replaced by '$\varphi$'. For simple mass transfer $0 \leqslant P_T \leqslant 1$, whereas if chemical reactions occur $-\infty \leqslant P_T \leqslant \infty$. Eq. (1) may be applied to enthalpy and momentum as well as chemical species. A variety of laminar and turbulent mass transfer problems, with or without heat transfer (including radiation), phase change, and chemical reactions were considered in Spalding's book on convective mass transfer [9], which was published 3 years later. The methodology was subsequently adopted by many others, and remains a standard approach in the engineering curriculum to this date; see, for example, [11,12]. An important point is that the methodology is appropriate for all convection–diffusion systems, i.e., a general system of conserved properties, and combinations of such variables.

Around 1960, Spalding had a simple but far-reaching idea [13]. Superficially this may have seemed a relatively unimportant contribution, yet it actually underlined his ability to apply a fresh direction of thinking to everything he touched. From the 1930s, research workers had been attempting to provide a continuous formula for the variation of mean velocity in the vicinity of a smooth surface where, for simple shear flows, $u^+ = f(y^+)$. Immediately next to the wall, in the viscous sublayer, the variation was assuredly linear and in the fully turbulent region for $y^+ > 30$ a logarithmic variation was accepted. But what of the region in between, sometimes called the buffer layer? The usual route at the time was to employ piecewise fits to different segments of the region. It was not easy to come up with a single analytical expression for the whole universal velocity profile. Spalding's contribution was to express the dimensionless distance $y^+$ as a function of the dimensional velocity $u^+$ (instead of the usual practice of writing $u^+$ in terms of $y^+$). The logarithmic part could be easily inverted as $y^+ = (1/E)\exp(\kappa u^+)$, where $E$ and $\kappa$ are constants. To complete the expression, he added to the right-hand side the laminar term $u^+$ and then subtracted a few terms from the power-series expansion of the exponential function. The resulting expression did have the correct asymptotic behaviour (linear and logarithmic) at very small and very large values of $u^+$ and did beautifully represent the transition layer as well.

A useful outcome of the above-mentioned analytical expression was that we could obtain an analytical expression for $dy^+/du^+$, which could then be easily related to the dimensionless turbulent (or effective) viscosity. Thus,

$$\frac{\mu_{eff}}{\mu} = \frac{dy^+}{du^+} = 1 + \frac{\kappa}{E}\left[\exp(\kappa u^+) - 1 - \kappa u^+ - \frac{(\kappa u^+)^2}{2} - \frac{(\kappa u^+)^3}{6}\right] \quad (2)$$

where the first term on the right-hand side represents the laminar contribution, while the rest is due to turbulence. Once the effective viscosity was expressed this way, it was possible to extend the idea to get an expression for the effective thermal conductivity

$$\frac{\Gamma_{eff}}{\mu} = \frac{\mu_{eff}/\mu}{\sigma_{eff}} = \frac{1}{\sigma} + \frac{1}{\sigma_t}\frac{\kappa}{E}\left[\exp(\kappa u^+) - 1 - \kappa u^+ - \frac{(\kappa u^+)^2}{2} - \frac{(\kappa u^+)^3}{6}\right] \quad (3)$$

where $\sigma$ and $\sigma_t$ are the laminar Prandtl number and the turbulent Prandtl number, respectively, and $\sigma_{eff}$ is the effective Prandtl number.

Using this framework, Spalding proposed that a thermal boundary layer growing through an already established velocity boundary layer (in a turbulent flow) can be calculated downstream of a discontinuity in wall temperature. This was published in Ref. [14], where he initially set the turbulent Prandtl number to unity. The key idea in this paper was used by Kestin and Persen [15], Gardner and Kestin [16], and Smith and Shah [17] to produce extensive numerical solutions for a range of Prandtl numbers and for both wall-temperature and heat-flux boundary conditions.

In a later paper [18], Spalding examined these solutions, discovered a regularity in them, provided approximate analytical formulas for them, and introduced the idea of a non-unity turbulent Prandtl number. He suggested that $\sigma_t = 0.9$ was more appropriate. This paper made another significant contribution. Since the influence of the laminar Prandtl number is limited to the region near the wall, the solutions for different values of the laminar Prandtl number behaved identically once the thermal boundary layer became thicker than the laminar sublayer. Thus, Spalding proposed that the only effect of the laminar Prandtl number was in providing an "extra resistance of the laminar sublayer". This resistance resulted from the fact that the value of the laminar Prandtl number was different from the value of the turbulent Prandtl number.

In terms of the relevant dimensionless variables, it was possible to write $dT^+/du^+ = \sigma_{eff}$. Therefore,

$$T^+ = \sigma_t \int_0^\infty \left(\frac{\sigma_{eff}}{\sigma_t} - 1\right) du^+ \quad (4)$$

This expression was considered to be valid for $u^+$ values beyond the laminar sublayer, where the effect of the laminar Prandtl number has all but vanished. This consideration allows the upper limit of the integral to be set to $\infty$, since the integrand falls to zero for large values of $u^+$.

Spalding identified this integral as the resistance of the laminar sublayer and called it the $P$ function, which depends only on the ratio $\sigma/\sigma_t$. Jayatilleke [19] working with Spalding, developed a comprehensive set of formulae for $P$ functions for smooth and rough walls in turbulent flows. The most commonly used of these expressions is

$$P = 9.24\left(\left(\frac{\sigma}{\sigma_t}\right)^{3/4} - 1\right)(1 + 0.28\exp(-0.007\sigma/\sigma_t)) \quad (5)$$

For moderate Prandtl numbers, this expression is sometimes simplified to: $P = 9.0(\sigma/\sigma_t - 1)(\sigma/\sigma_t)^{-0.25}$. This function is widely used to this day to provide the wall boundary condition in turbulent flow calculations.

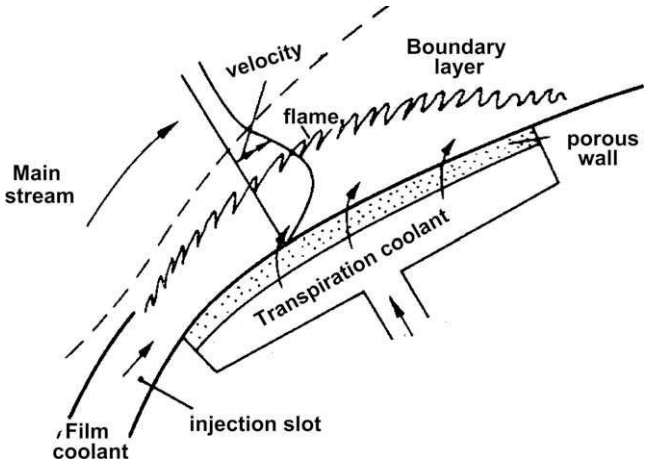


**Fig. 1.** Illustration of the type of process which was considered. From Ref. [22] with permission.

## 4. The Unified Theory

In his book Convective Mass Transfer [9], Spalding sought to unify heat transfer and mass transfer. He also considered simultaneous heat and mass transfer (including evaporation, ablation, and combustion) in a single framework. Around the same time, he became fascinated by the Russian book by Kutateladze and Leontev, which he translated [20].

In the Preface to the translation, he wrote:

> "*No previous textbook authors have been bold enough to recommend methods for calculating drag and heat transfer under conditions of high Mach number, pressure gradient, and simultaneous mass transfer... The authors have set a standard of comprehensiveness which will be both an inspiration and a challenge to later workers.*"

It seems that Spalding himself accepted the challenge and set out to create a single calculation method for turbulent shear layers (including boundary layers, jets, wakes, wall jets, and duct flows) in the presence of pressure gradient and mass transfer. This is what came to be known as the Unified Theory. Unification of Flow, Heat and Mass Transport was to stay as the dominant theme of his research throughout his professional career and has had a significant impact on the CFD community.

In 1964, Spalding published an Aeronautical Research Council Report [21] with the title "A Unified Theory of Friction, Heat Transfer and Mass Transfer in the Turbulent Boundary Layer and Wall Jet". In December 1964 the report was retyped and annotated [22]: there were 87 typed foolscap pages and 29 figures. It was the true start of the extraordinary contributions made by Spalding to the prediction of turbulent shear flows. As if the title were not ambitious enough in scope, Fig. 1 of the paper (reproduced here) revealed the extent of his vision although, as he makes clear on p. 1 of the paper, not all the features represented are usually present simultaneously. Remarkably, the paper was never published in a refereed journal even in an abbreviated form. A possible explanation is that developments were moving so rapidly, both within his own group and elsewhere, that Spalding had decided the Unified Theory would be superseded very quickly and was not worth pursuing further.[2]

[2] Spalding himself commented recently that he felt the paper was "too short for a book and too long for a journal paper".

On p. 4 we read

*"The new theory rests on two main postulates. The first is that the velocity, temperature and concentration profiles can be described by formulae having two main components, one accounting for effects of momentum, heat and mass transfer to the wall, and the other accounting for interactions with the main stream; thus the general profiles have both "boundary-layer" and "jet" components. The second is that fluid is entrained into the wall layer in the same manner that it is into a turbulent jet and in accordance with similar quantitative laws."*

It is interesting to note that prior to the Unified Theory (UT), Spalding's publications indicated little interest in turbulent flows, although the 1961 paper by Ricou and Spalding [23], which was concerned with entrainment by turbulent jets, is a notable exception. Spalding went on to say that once the "new" theory had been conceived it soon became apparent that its elements were not new at all. He suggested that it might be helpful to regard the Unified Theory as a combination of the velocity-profile formulae of Coles [24] and others with the entrainment hypothesis of Head [25] (although that was not the genesis of the theory).

The theory was developed in detail in Section 2 of the report. The integral forms of the boundary-layer equations for momentum and a conserved property were written and the velocity profile represented "*with sufficient accuracy*" by the relation

$$z = s^{\frac{1}{2}}u^{+}(y^{+}) + (1 - z_E)(1 - \cos \pi\xi)/2 \tag{6}$$

where $z = u/u_G$ is non-dimensional velocity, $u_G$ being the free-stream velocity, with an appropriate form for the wall function $u^+(y^+)$ to include the effects of mass transfer. The key feature of this equation, which is very close to the well-known relation proposed by Coles, is the appearance of the parameter $z_E$ which, it was said, "*will assume great importance later*". An analogous equation was introduced for the conserved property $\varphi$ which could stand for the composition of a chemically inert component of a mixture, stagnation enthalpy, etc. A preliminary entrainment law was then introduced guided by information about the plane free turbulent mixing layer. Head had attempted to correlate the entrainment rate with a shape factor $H_l$, defined as $(y_G - \delta_1)/\delta_2$, $y_G$ being the velocity boundary-layer thickness whereas Spalding, displaying his usual physical insight, realized that the entrainment rate was more likely to be proportional to $(1 - z_E)$, the strength of the jet or wake component of the velocity profile. In fact in the original Unified Theory [21] he developed a more complicated pair of equations

$$\begin{aligned} z_E < 1 &: -m_G = 0.1023(1 - z_E)\left(1 + \frac{1}{3}z_E\right) \\ z_E > 1 &: -m_G = 0.09(z_E - 1)\left(1 + \frac{1}{3}z_E\right)/(1 + z_E) \end{aligned} \tag{7}$$

wherein $-m_G$ is the non-dimensional entrainment rate. Both equations were later simplified by Spalding [22] as they were thought to be over-elaborate and found to over-estimate entrainment rates and were modified further by him shortly thereafter [26]. The Unified Theory was shown to be consistent with many other aspects of turbulent boundary-layer theory and, indeed, showed how a unified approach could be developed to encompass such influences as heat and mass transfer, roughness, and even property variations.

The responsibility for developing the purely hydrodynamic aspects of the Unified Theory for constant-property boundary layers was given to two research students, Escudier and Nicoll. Analysis of experimental data available in the literature for turbulent boundary layers ($z_E < 1$) was carried out by the former while the latter was concerned with wall jets ($z_E > 1$) where few data were available and so extensive experimental work was required. Entrainment rates were derived using the formula

$$-m_G = \frac{dR_m}{dR_x} \tag{8}$$

where $R_m = \int_0^{y_G}(u dy/v)dy$ and $R_x = \int_0^x (u_G dx/v)dx$. Although $y_G$ was estimated systematically by fitting the velocity-profile equation to measured data, the uncertainty inherent in this procedure was obvious. A computer program was developed to predict boundary-layer and wall-jet development based on the Unified Theory. This code was programmed, originally on punched five-hole tape and later IBM cards, and ran on the University of London Atlas[3] computer. The outcome of the Escudier–Nicoll collaboration was presented in [27], in which the final version for the entrainment rate equations was

$$\begin{aligned} z_E < 1 &: -m_G = 0.075(1 - z_E) \\ z_E > 1 &: -m_G = 0.03z_E - 1 \end{aligned} \tag{9}$$

Extensive calculations were presented and discussed with the final conclusion that "The boundary-layer predictions are in reasonable agreement with experiment, except where separation conditions are approached" and "The wall-jet predictions are good, both for zero pressure gradients and for adverse pressure gradients". On the other hand Escudier and Nicoll gave the usual explanation for the poor performance for adverse-pressure-gradient boundary layers, namely, to blame the experimental data for not satisfying the two-dimensional condition. There is some truth here; see Fellouah and Pollard [28].

It has already been mentioned that in the year following publication of the Unified Theory, Spalding modified the equation relating the non-dimensional entrainment rate, $m_G$, to the wake parameter $z_E$ [26]. In fact, it was in the latter paper that Spalding first considered an approach to boundary-layer prediction based upon solution of the momentum-integral equation and the kinetic-energy-deficit equation of the turbulent boundary layer. He showed that there was a formal relation between the entrainment function, $m_G$, and the dissipation integral, $\bar{s}$, which appeared in the well-established theories of Rotta [29] and Truckenbrodt [30]. He went on to recommend improved, but provisional, expressions for $\bar{s}$ valid for $z_E < 1$, including near-separating boundary layers, and for $z_E > 1$. Spalding stated "*The author's present opinion is that it will ultimately be preferable to use the "kinetic-energy" method rather than the "mass-conservation" method*". His reason was 'the greater directness with which $\bar{s}$ can be connected with density-variation, radius-of-curvature and other effects'. It is clear that the entrainment approach was to all intents and purposes history in the eyes of Spalding by 1965: he says "*it should not be forgotten that the role of the entrainment-based theory, although perhaps brief, was a valuable one*", but there was no hint that the dissipation-integral approach was also doomed to be short lived.

## 5. From unified theory to computational fluid dynamics

By 1965, UT was well established and it was Spalding's prime focus and his expectation that UT would be generally valid for a very broad range of flows beyond the so called "boundary" layer flows. UT was a "grand design" built upon the insights of Taylor [31] to have a single theory that covered the canonical flows of boundary layers, wakes and jets. The essence was the use of classical profile methods which had been perfected by Polhausen and others. Spalding was aware that the profile methods, then in vogue, had severe limits. An analytical profile had to be devised that represented the flow well, and had the right number of parameters to

[3] http://www.chilton-computing.org.uk/acl/technology/atlas/overview.htm.

satisfy the initial and boundary conditions. This was a demanding and complex task. Spalding therefore proposed to generate universal profiles by representing them with piece-wise segments and then derive the matching constants from the initial and boundary conditions and other mathematical constraints. Although in principle any profile could be used, Spalding decided to rely on simple linear or polynomial segments. Such a piece-wise profile could approximate to a given accuracy any ideal profile that might describe the flow. He worked towards it with a series of students and had a fair amount of success. His previous students had already determined optimal entrainment functions, log-law constants, and heat and mass transfer resistance required to describe a wide range of flows. A research student, S.V. Patankar, had a positive outcome on the theoretical side in building a general purpose "integral-profile" computer code based on piece-wise linear segments.

Prediction of the hydrodynamic aspects of boundary-layer flows, based on solution of the momentum and kinetic energy equations, was later extended to the temperature equation by using two parameters for the temperature profile: the thermal boundary-layer thickness and a wake-like parameter. These were obtained from the energy equation and a "T-squared" equation, which was the counterpart of the kinetic energy equation. This was published at the 1966 International Heat Transfer Conference in Chicago [32]. At this time, Spalding effectively started using the idea of weighting functions. The kinetic energy equation and the "T-square" equation did not require a physically understandable basis; they could be considered as integrals of the momentum and energy equations after multiplication by a weighting function (which could be the dependent variable itself). In the search for greater flexibility and wider applicability, many families of weighting functions were considered. For example, the use of powers of $u$ (or $T$) led to the kinetic energy and related equations. Powers of $y$ (as weighting functions) led to various "moment of momentum" equations. Another option was to use subdomain weighting functions. With so many integral equations available, the profiles could now have a large number of parameters; they could be polynomials, or better still, piece-wise linear. During this time of exploration, Spalding also suggested a variety of independent variables for the cross-stream coordinate in the boundary layer. The distance $y$ or the dimensionless distance $y/\delta$ were the obvious candidates; but he suggested the stream function (and its dimensionless counterpart), which simplified the representation of the cross-stream velocity or flow rate.

Spalding was at that time confident that many flows of engineering interest could be represented by his unified theory and the piece-wise profiles. Although the theory had produced a number of remarkable advances, flows with strong favourable or adverse pressure gradients remained outside the scope of UT. Such flows included important classes of industrial flows such as wall jets and separated flows, including flow behind a pipe step or over a cavity. The major problem with the unified theory was the need to calculate profile parameters, using a set of algebraic equations. These equations could develop singularities, e.g., in the transition of a wall jet to a boundary layer.

Shear plays a key role in separated flows, including those where the boundary layer is destroyed by, say, an adverse pressure gradient, or a geometry that induces separation. Since the core of UT relied on the parabolic version of the Navier–Stokes equations, such flows were outside the scope of UT. Spalding's idea was that profiles would be found that could evolve and represent these flows which otherwise had no "self-similar" behaviour. He therefore assigned two new students to tackle the problem of bringing such flows within the scope of the unified theory: Wolfshtein had already joined the group in August 1964 and Spalding asked him to tackle the problem of the impinging jet on a flat plate; flow behind a backward-facing step in a channel and that in a driven-lid square cavity were to be the focus of attention for Runchal. These extensions would have firmly established the Unified Theory not only for parabolic flows such as the boundary layers but also for elliptic flows with strong pressure gradients, recirculation and impingement. By the end of 1965, from the preliminary work of Runchal and Wolfshtein, it became apparent that UT had two serious shortcomings as far as separated or high pressure gradient flows were concerned. The underlying structure of UT was the parabolic Navier–Stokes equations and included an inherent assumption that "self-similarity" existed. Spalding realized that the UT and the profile method had a fatal flaw. There was no easy way to represent the role of the axial diffusion that destroys the self-similarity and plays a key role in separated and reversed flows. The UT could not be extended to such flows. During this attempt to extend the UT to strong pressure gradient flows, it also became apparent that the only general method then available to tackle the full (elliptic) form of the Navier–Stokes equations was the method of finite differences. In one way the finite difference method (FDM) was similar to the central idea of the Unified Theory: both used piece-wise polynomial profiles. But there was an essential difference also. While UT relied on solving for the matching constants that completed a profile, the FDM used a simple universal piecewise profile to solve directly for the value of the governing variable. In essence there is no explicit profile beyond the immediate neighbourhood of the point of interest (or node) in the computational domain. This may be thought of as a locally evolving profile rather than a generic profile.

Finite difference methods for Navier–Stokes equations have been around for a long time: Thom [33] had used them well before the advent of electronic computers and Burggraf [34] had more recently applied them to a separated flow in a square cavity. It became apparent that it would be simpler and more general to use the FDM method rather than to modify the UT. In January 1966, Runchal and Wolfshtein combined their individual research goals and started writing a general purpose FDM computer program. Since their immediate interest was in solving two-dimensional problems, the stream function–vorticity ($\psi$–$\omega$) form of the Navier–Stokes equations was the focus of their attention. The $\psi$–$\omega$ approach eliminates pressure from the equations and also results in a set of two rather than three coupled partial differential equations. Early on, it became apparent that there were limitations of the standard, and then preferred, option of using central differences for FDM. The solution failed to converge for high Reynolds number flows. Stability analysis showed that this was because the matrix coefficients were no longer positive-definite at high Reynolds numbers. Spalding then made the analogy of how the wind from the pigsty always stinks – or that northerly winds (in the Northern hemisphere) generally bring the cold. These discussions led to the development and use of the "upwind" concept. It later turned out that one-sided differences had been previously used by Courant et al. [35] and others. The important contribution made by Spalding, was the adoption of the concept of a finite-volume method (FVM) as the core of mathematical development rather than the use of the traditional FDM.[4] Spalding likened the computational grid to a series of 'tanks' (that hold the nodes) and the 'tubes' (that convey the fluid along the grid). These improvements rapidly led to success. By June of 1966, Runchal and Wolfshtein reported results both for the wall jet and for the separated flows behind a backward-facing step and in a driven-lid square cavity for low and high Reynolds number flows. This was reported in a series of papers from Imperial College [36–39]. By late 1966, the method

[4] It was not until some time later that the terminology "finite volume" was adopted.

was well established and began to be used widely by other researchers all over the world. It was subsequently published in book form by Gosman et al. [40].

One shortcoming of the $\psi$–$\omega$ method was that it was essentially limited to two-dimensional flows and could not easily be extended to three dimensions in any obvious manner. The possible extension using the vector vorticity and the vector velocity potential (which is the counterpart of the stream function) was thought at the time to be far too complicated; it was feared that the delightful simplicity in the two-dimensional arena would simply go away and as a result further advances (as documented below) were based on the so-called primitive variables, namely the velocity components and pressure. However, the vorticity–vector potential formulation was in fact later successfully used by Mallinson and de Vahl Davis [41] and many others.

With the development and the success of the FVM and the inability to extend the UT to flows with strong pressure gradients, the progression of UT (based on integral equations) came to an abrupt halt in the summer of 1966 when Spalding travelled with Patankar to the 1966 International Heat Transfer Conference in Chicago to present a paper on their work on the UT [32] and to work on a consultancy project for the summer break. During this period, with the already demonstrated success of the FDM for elliptic flows at the back of their minds, they decided to essentially abandon the "piece-wise-profile" method for UT and switched over to FDM for the parabolic form of Navier–Stokes equations for two-dimensional boundary layers. They introduced the innovation of replacing the distance normal to the wall by a non-dimensional stream function based variable – essentially the von-Mises transformation – as the cross-stream coordinate, a piecewise-linear profile for velocity (and temperature), and the subdomain weighting function. Suitable entrainment formulas were used at free boundaries to determine the growth of the calculation domain into the surrounding free stream. This method had the speed, flexibility, accuracy, and simplicity needed for a general procedure for two-dimensional boundary layers, free-shear flows, wall jets, and duct flows.

Thus by the end of 1966, both the elliptic and parabolic FDMs were firmly established and the entire focus of the group shifted to application and improvement of this technology. With the publication of the papers [42,43] and later the books by Patankar and Spalding [44,45] and Gosman et al. [40] both the elliptical and the parabolic methods gained considerable following and were widely used by researchers at Imperial College, Stanford University, and elsewhere. A number of Ph.D. theses applied the methods to a variety of parabolic and elliptic flows. This was also the time when research on mathematical models of turbulence was in full swing. The CFD codes provided a convenient vehicle for testing turbulence and combustion models. The two-flux and six-flux models for radiation [46] and formulations for particle concentrations in different size ranges were also implemented in the framework of these methods.

By 1968, evidence began building up that for many applications the FDM and FMV with upwind differences led to undue false (numerical) diffusion. The effort therefore shifted to finding superior methods for representing the convective terms. A number of higher order schemes, including the concept of vector-differencing following the stream-lines, were explored, although none proved entirely satisfactory. Spalding [47] then proposed an exponential method to replace upwinding, but eventually the Imperial College group settled on a "hybrid" difference scheme [48] that blended the central and upwind difference methods based on the local Péclet number. For quite some time this [40,43] became the standard approach for solving high Reynolds number flows, but was later augmented by higher order upwinding, QUICK [49] and vectored upwinding schemes, and by the use of fluxes, not profiles of variables.

It was realized that the "tank-and-tube" approach could be replaced by the Gauss Theorem. This avoids the use of the Taylor series and leads to an elegant formalism to derive the discrete set of equations in any arbitrary shaped control volume. This generalized FVM revolutionized the engineering practice by giving rise to the new field of computational fluid dynamics (CFD). General and flexible computer codes could be written to solve fluid flow problems in any complex geometry at any Reynolds number. In an important way the FVM also changed the basic thinking behind computational fluid dynamics. Unlike the mathematical approach used by FDM and the finite element method (FEM), an understanding of the FVM was enhanced by a physical approach to the problem. The focus of interest was not the variable and its interrelationship parameters with other nodes; the focus now was on the control volumes and the fluxes crossing their boundaries and the sources or sinks contained within them.

Further research, and the continued creativity of Spalding, led to a new and improved version of the parabolic boundary layer method, which was published in the 1970 edition of the book by Patankar and Spalding [45]. This contained a new computer program called GENMIX. In 1977 Spalding published a book [50] which is in the nature of a user manual for GENMIX. The method now included an improved way of calculating the entrainment and a procedure for determining the unknown pressure gradient in confined flows. The new method now contained the hybrid scheme developed earlier for the elliptic model for high Reynolds number flows.

The parabolic boundary layer procedure of Patankar–Spalding was based on a non-iterative scheme that employed a purely "marching" procedure. Spalding explained the non-iterative determination of the pressure gradient in a confined flow via a 'car-steering analogy'. The calculation of the entrainment at the free boundaries also remained a source of oscillations and instability in many applications of the method. Formally, the equations are nonlinear and an iterative solution would have addressed this in a forthright manner. (Later in the general-purpose CFD code PHOENICS, described below, Spalding [51] addressed these issues and did employ iteration at the forward step.) The entrainment rates (and the unknown pressure gradient in a confined flow) should have been recognized as eigenvalues in the equations to be determined from certain overall properties of the resulting solution. With what we know now, a much more robust and efficient procedure for two-dimensional boundary layers could now be constructed; but there is hardly an incentive to develop such a method in this day and age.

In 1967 Spalding made a contribution that on the face of it seems trivial but had a profound influence on later thinking and development of CFD tools. He introduced the concept of a "General Transport Equation" to express all second order convective-diffusive transport equations. He proposed to write them as a single equation for a generalized variable $\varphi$ that represented velocity components, enthalpy, or chemical species. This generalized transport equation has four components: (1) transient or accumulation, 2) convection, (3) diffusion, and (4) source term. Thus the Navier–Stokes, energy and mass (species) transport equations could all be expressed by this single equation:

$$\frac{\partial}{\partial t}(\rho\phi) + \mathrm{div}(\rho\mathbf{u}\phi) = \mathrm{div}(\Gamma\ \mathrm{grad}\ \phi) + S \tag{10}$$

Early examples of this formulation appear in the 1969 book by Gosman et al. [40]. This was his effort at "unification" of mathematical expression. This approach led to the fast development of CFD methodology since one can concentrate efforts at solving this single equation rather than look at the specifics of each variable.

Another innovation that Spalding introduced around 1966 was that of the "compass" notation to express the FD or FV stencil. This simplified the visualization and expression of the fluxes and

meshed in with his "tank-and-tube" approach to FV. The six points (or control volumes) surrounding a central point (or CV) were designated "north", "south", "east", "west", "high", and "low". Thus, the "standard" form of the linear algebraic equations, written in the so-called zero-residual form, is

$$a_W(\phi_W - \phi_P) + a_E(\phi_E - \phi_P) + a_S(\phi_S - \phi_P) + a_N(\phi_N - \phi_P) + a_L(\phi_L - \phi_P) + a_H(\phi_H - \phi_P) + S = 0 \quad (11)$$

By 1969, the interest of the Imperial College group began to shift to three-dimensional flows. The stream function–vorticity variables had distinct advantages for two-dimensional flows but, as previously mentioned, their use for three-dimensional flows was problematic. After some preliminary ($\psi$–$\omega$) extension to such flows, Spalding started to look for methods based directly on the primitive form of the Navier–Stokes equations. A number of alternatives were tried but none proved entirely satisfactory. The first hint of success came with the coupled SIVA scheme of Caretto et al. [52]. However the coupled scheme was deemed to be computationally expensive and the focus shifted to the search for an efficient sequential or segregated method of solving the governing equations. By this time Harlow and co-workers [53] had demonstrated the advantages of a staggered grid algorithm and Chorin [54] had published work on pressure splitting (or pressure projection) algorithms. Patankar and Spalding [55] combined these ideas with the FVM technology and hybrid-differencing developed earlier to arrive at a robust and general 3D Navier–Stokes solver called SIMPLE (Semi-Implicit Method for Pressure-Linked Equations). The SIMPLE algorithm went on to achieve a classic status, and led to the commercialization of the new CFD technology.

## 6. The SIMPLE algorithm

Around 1970, there was an effort to develop a procedure for three-dimensional boundary layers (or three-dimensional parabolic flows). It was quickly realized that this was not a simple or straightforward extension of the two-dimensional boundary layer procedure. The three-dimensional boundary layer contained within it a parabolic behaviour in the streamwise direction and an elliptic behaviour in the cross-stream plane. For this "elliptic" problem, the stream function–vorticity procedure could not be used because the three-dimensionality of the flow precluded the use of the stream function as a variable. The obvious choice was to use the velocity components directly.

The breakthrough contribution by Spalding was the identification of the role of the pressure gradient. To preserve the marching nature of the solution procedure for this parabolic problem, Spalding required that the streamwise momentum equation was driven by a single pressure gradient $dp/dx$ across the whole boundary layer at a given $x$. This pressure gradient could be obtained from the pressure gradient in the external free stream (for unconfined flows) or from the overall mass conservation (for confined flows). Then the cross-stream velocity components were governed by their momentum equations and a pressure variation in the cross-stream plane that was needed to satisfy the local continuity equation. Although this pressure variation in the cross-stream plane was calculated, it was not used in modifying the streamwise pressure gradient $dp/dx$ used for the streamwise momentum equation. Thus, an inconsistency was deliberately accepted in the treatment of pressure. Spalding maintained that this inconsistency was a small price to pay for the benefit of using the marching procedure for the parabolic flow. In practice, the cross-stream variation in pressure would be rather small and no significant error was involved.

If this was an important issue, why did we not know about it while studying the two-dimensional boundary layer? Do the solutions for the two-dimensional boundary layer contain the same inconsistency about pressure? Spalding was able to point out that the issue was present all along in the two-dimensional boundary layer, but remained invisible; it is the three-dimensional boundary layer that brought the issue to the forefront.

In a two-dimensional boundary layer, we obtain the streamwise velocity by solving the streamwise momentum equation, in which we use a single value of $dp/dx$. Then we obtain the cross-stream velocity from the continuity equation. The cross-stream momentum equation does not get used at all! If we were to use it, we would be able to calculate the variation of pressure in the cross-stream direction, thus exposing the inconsistency with the value of $dp/dx$ used.

In a three-dimensional boundary layer, there are two cross-stream velocities. The continuity equation alone cannot determine these two velocity components. How the flow distributes in the two cross-stream directions is decided by the variation of pressure over the cross-stream plane. We are forced to solve the cross-stream momentum equations and calculate the variation of pressure over the cross-stream plane. The pressure inconsistency cannot be hidden under the carpet!

The *S*emi-*I*mplicit *M*ethod for *P*ressure-*L*inked *E*quations (SIMPLE) was described in the paper by Patankar and Spalding [55]. The main ingredients of the method are:

- calculation of the streamwise velocity component by solving the streamwise momentum equation with a value of $dp/dx$ that remains the same across the cross-stream plane
- calculation of the cross-stream velocity components and cross-stream pressure variation by solving the cross-stream momentum equations and continuity.

The latter step required the development of a new algorithm, which is the heart of SIMPLE. It was recognized that we could always solve the momentum equations for any specified pressure field; but then the resulting velocity field would not normally satisfy the continuity equation. We could then propose "corrections" to the specified pressure field so that the resulting (corrected) velocities would satisfy continuity. This led to the birth of what was called the "pressure correction equation". It was actually a rewritten form of the continuity equation, which gave a direct means of calculating the pressure corrections (and hence the pressure).

Although in the 1972 paper, Patankar and Spalding presented the SIMPLE algorithm in the context of three-dimensional parabolic flows, it was obvious that the method contained within it a procedure for two-dimensional elliptic flows, since that is how the cross-stream velocities were treated. Further, the method could easily be extended to three-dimensional elliptic flows, as it did not rest upon any concepts (such as the stream function) that were specific to a two-dimensional situation. Thus, SIMPLE provided a general calculation procedure for solving the coupled momentum and continuity equations in any dimensionality. Once again, this method became very widely used all over the world. Improved variants of the method, such as SIMPLEC [56], SIMPLER [57], and SIMPLEST [58] were later developed by different researchers, in part to strengthen the coupling between velocity and pressure and provide more robust algorithms with faster convergence.

## 7. Multi-phase flow

During the mid and late 1970s, Spalding began extending SIMPLE-like methods to multi-phase flows. The *I*nter*P*hase *S*lip *A*lgorithm, IPSA, is the two-phase Eulerian–Eulerian algorithm which

Spalding pioneered [59,60]. It is a natural and elegant extension of the single-phase SIMPLE algorithm. Although in its original formulation and the description below, only two phases were identified, all the main ideas are easily extendable to multi-phase (i.e., more than two) flows. It first appeared in 1977 at an ICHMT Seminar in Dubrovnik, see Spalding [60].

Spalding considered a two-phase flow as composed of two interpenetrating and intermingling continua. Each location (and as a result, each finite-volume cell) potentially had both phases (e.g., liquid and gas) present. The amount of each phase was characterized by its volume fraction. Such a model of two-phase flow does not describe how the two phases are locally distributed. The volume-fraction characterization cannot distinguish between large chunks of liquid and fine droplets. It is this characterization that leads to the simplicity of the formulation and also to its main weakness. Spalding later presented extensions for removing this weakness [61].

For the two interpenetrating continua, he proposed two sets of conservation equations for the phases. These were similar to the single-phase equations, except for an additional pair of inter-phase transport terms. Thus, the velocity difference between the two phases at a point would lead to a force term due to the shear force exerted by one on the other, and temperature difference between the two phases would lead to an inter-phase heat transfer. The inter-phase transport strongly depends on the surface area available for shear or heat transfer. This in turn requires the size of the droplets of the particulate phase. The volume-fraction characterization does not provide this information. Indeed the multi-phase flow problem is a classic example of a closure problem, of which turbulence is, perhaps, the example best known to the engineering student.

It seemed practical to solve the conservation equations for the two phases in a segregated manner; that is, to solve for the velocities and temperatures of one phase followed by those for the other phase. Thus, while solving for one phase, the values of velocity and temperature for the other phase were assumed to be known from the previous iteration. When inter-phase transport was dominant, this procedure would converge very slowly since the assumed values of the other phase would dominate the behaviour of the current phase. Spalding had already seen this problem in another context. In a heat exchanger analysis, discussed elsewhere in this article, the temperatures of the shell-side fluid and the tube-side fluid influence each other in the same manner. Spalding thus invented the *P*artial *E*limination *A*lgorithm (PEA) precisely to handle such a situation. The trick was to solve the equations for temperature in an algebraically transformed form that eliminated the direct contribution of the 'other' temperature. (There are still some terms that indirectly contain the neighbour values of the 'other' temperature, which is why the transformation is partial and not total.) The reduction of the influence of the 'other' temperature (or velocity) gave an impressive speedup of the iteration process. Spalding immediately identified the two-phase flow problem as a candidate for PEA. It turns out that the use of the PEA is essential for the success of most two-phase flow calculations. A 'sum-to-unity' requirement was also imposed and ensured that the coupling between the phase volume fractions is preserved at all times during the solution procedure.

If the overall continuity equation is written as a mass-conservation equation, the terms for the denser fluid (liquid) excessively dominate the terms for the lighter fluid (gas). To overcome this difficulty, Spalding wrote a ''volume continuity equation" [62] which gave comparable weighting to the two phases. The *G*as *A*nd *L*iquid *A*nalyser (GALA) employs volumetric rather than mass continuity, and is advantageous for computing the movement of fluids containing discontinuities of density, especially those of large magnitude such as between a gas and a liquid. This overall continuity equation forms the basis of creating the pressure or pressure correction equation for two-phase flows. Although the notion of a single 'shared' pressure is fundamental to the procedure, IPSA permits there to be two different fluid pressures, provided an appropriate algebraic relationship between the two individual pressures is known. Thus, the phase continuity equations are used to obtain the volume fractions of the individual phases and, by analogy to SIMPLE, overall continuity is converted to a pressure correction equation.

Like SIMPLE, IPSA was rapidly adopted by researchers around the world, and variants of IPSA form the basis for two-phase Eulerian–Eulerian formulations in almost all multi-phase finite-volume CFD codes today. The basic framework for two-phase flows was later extended, conceptually, to multi-phase flows of various kinds, using the 'algebraic-slip method' (sometimes called the mixture model or drift-flux model). In essence, the algebraic slip model is comprised of continuity and momentum equations for the mixture, continuity equations for the dispersed phases, and algebraic relationships for the slip velocities. One could consider liquid droplets in different size ranges, gas packets of different concentrations, and so on. In the subsequent implementation of IPSA in the PHOENICS code, a phase-diffusion term was also included in the phase continuity equations. Spalding modelled this term by means of a gradient diffusion assumption so as to represent the turbulent flux associated with correlations between fluctuating velocity and volume fraction. Some later researchers argued for excluding the phase-diffusion term in favour of a turbulent dispersion force in the momentum equations, e.g., Lahey et al. [63]. The phase-diffusion terms proved to be an important element in some variants of Spalding's two-fluid model of turbulence, Malin and Spalding [64]. Later, (i.e., post 1980), Spalding used the two-phase concepts to devise advanced turbulence models [64–67] (considering the turbulent flow as a two-phase mixture of laminar and turbulent chunks) and advanced combustion models [68–70] (considering a mixture of reacted and unreacted gases).

## 8. Turbulence modelling

With the development of the Patankar and Spalding [42,44,45] finite-volume solver for two-dimensional thin shear flows, the need (so far as turbulence modelling was concerned) shifted to providing a route for determining the effective turbulent stresses and heat fluxes throughout the computational domain, a problem that Spalding simplified to that of obtaining the local turbulent viscosity. The initial model in the Patankar–Spalding method was Prandtl's mixing-length hypothesis, a scheme employed in several early papers including his group's submission for the Stanford Conference, Kline et al. [71].

Spalding's vision, however, was already on providing a corresponding computational procedure for recirculating flows and here he recognized that the mixing-length scheme was quite inadequate. In Ref. [72], he sets out to explain why, in a separated flow, the wall heat flux often reaches a maximum at the reattachment point. As he remarked [72]

> ''*This fact assumes particular interest when it is recalled that, at the reattachment point, the (time-mean) shear stress is zero; and most formulae for calculating heat transfer rates which are based on a physical theory of flow in a boundary layer would predict that, where the shear stress is zero, the heat transfer must also vanish*."

The apparently paradoxical behaviour of separated flows he explained as due to the diffusional transport of turbulence energy, $k$, towards the wall. He provided evidence for this assertion by carrying out an approximate analytical solution of the turbulence energy equation, showing that, with the empirical coefficients

appearing in the diffusion and dissipation terms chosen from quite different flow types, the observed power-law dependency between Stanton and Reynolds numbers was correctly reproduced. The turbulence energy equation had been employed over the preceding twenty years by several turbulence modellers, e.g., Prandtl [73], but Spalding's paper was the first to show an application of the equation to an idealization of a separated flow and how it resolved the question of why heat transfer in separated flows followed different rules of behaviour from those in boundary layers. It was presumably from this research that the decision was taken to embed the Prandtl–Glushko turbulence energy model into the slightly later numerical scheme for recirculating flows, Gosman et al. [40]).

A second major contribution, linked to the foregoing, concerned improving the near-wall logarithmic velocity profile (onto which the numerical solution for the outer region was fixed to avoid what, at the time, was the impossible numerical requirement – not to mention the modelling problems – of resolving the viscous sublayer in an elliptic solver). As noted above, Spalding recognized that the usual formula

$$u^+ \equiv \frac{u}{(\tau_w/\rho)^{\frac{1}{2}}} = \frac{1}{\kappa}\ln\left[\frac{Ey(\tau_w/\rho)^{\frac{1}{2}}}{\nu}\right] \tag{12}$$

and the corresponding temperature distribution

$$T^+ \equiv \rho(\tau_w/\rho)^{\frac{1}{2}}c_p\Delta T/q_w = (\sigma_t/\kappa)\ln\left[\frac{Ey(\tau_w/\rho)^{\frac{1}{2}}}{\nu}\right] + P(\sigma_t/\sigma) \tag{13}$$

were deficient in several respects in the vicinity of stagnation points simply because there, the friction velocity $(\tau_w/\rho)^{\frac{1}{2}}$ was an inappropriate velocity scale. Having shown the necessity of including the turbulence energy in computations of separated flows, he proposed that the dimensionless parameters appearing in the above law-of-the-wall formulae should be changed to:

$$u^* \equiv \frac{uc_\mu^{\frac{1}{4}}k^{\frac{1}{2}}}{(\tau_w/\rho)} = \frac{1}{\kappa}\ln\left[\frac{Ec_\mu^{\frac{1}{4}}k^{\frac{1}{2}}}{\nu}\right] \tag{14}$$

$$T^* \equiv \rho c_\mu^{\frac{1}{4}}k^{\frac{1}{2}}c_p\Delta T/q_w = (\sigma_t/\kappa)\ln\left[\frac{Ec_\mu^{\frac{1}{4}}k^{\frac{1}{2}}}{\nu}\right] + P(\sigma_t/\sigma) \tag{15}$$

The starred quantities introduce the turbulence energy, $k$. (In equilibrium, $u^*$, $T^*$ are the same as $u^+$, $T^+$, but not otherwise.)

The change from Eqs. (12) and (13) to Eqs. (14) and (15) simply involved replacing $\tau_w/\rho$ by $c_\mu^{\frac{1}{2}}k$. Indeed, the coefficient $c_\mu$ was chosen as 0.09 so that, in an equilibrium flow near a wall (where the wall shear stress is proportional to the turbulence energy in the "log-law" region), the formula gives the same results as the more traditional form, Eqs. (12) and (13). A further important feature of Eq. (14) is that the wall shear stress becomes directly proportional to the wall-parallel velocity which is important when the flow is close to separation. Spalding's version of the law of the wall was employed in software at Imperial College from the beginning of the 1970s and was finally published in the review paper by Launder and Spalding [74] to which further reference is made below. The form became, and remains, the standard wall treatment for most of the commercial CFD codes that have emerged over the past 30 years. Unlike the original law-of-the-wall, it always gives at least qualitatively correct heat transfer patterns in recirculating flows, although more reliable wall-function schemes are nowadays employed in research-level CFD.

Despite the very real benefits of introducing the turbulence energy to compute recirculating or other far-from-equilibrium flows, Spalding realized that, because the Prandtl–Glushko model (like the mixing-length hypothesis) needed an empirical specification of the turbulent length scale, it was extremely limited in its width of applicability. He saw that more general and more complete models required, in addition to an equation for $k$, a further transport equation for calculating the distribution of the turbulent length scale over the flow field. Inspired by the work of Kolmogorov [75] and Rotta [76] who proposed length-scale equations for the fluctuation frequency, $\omega$, and the product of $k$ and the length scale, $L$ (i.e., a $kL$-equation) respectively, Spalding pushed forward the development of models using such an equation, i.e., the development of two-equation models. In an early report [77] he used Rotta's length-scale equation in integral form to show that various free turbulent shear flows (notably the mixing layer, the plane jet, and the fan jet) could be calculated with the same set of constants, while, in contrast, the mixing-length model required different ratios of mixing length to flow width to give the correct rate of spread. Then, to support these findings by numerical calculations and to develop a general model for the computer codes his CFD team had created, he gave two Ph.D. students the task of developing and testing, with the aid of the Patankar–Spalding boundary-layer code, a model using Rotta's length-scale equation together with a transport equation for $k$ and the Prandtl–Kolmogorov eddy-viscosity assumption. Rodi performed the development and testing of the model for free flows while Ng took on the development and testing for near-wall flows. This research led to the establishment of the $k$–$kL$ model. In Rodi and Spalding [78], the superiority of this two-equation model over the mixing-length model was confirmed for free flows. This work also brought out the so-called plane/round jet anomaly, i.e., the fact that the plane and the round jets in stagnant surroundings cannot be calculated with a model with the same constants. The near-wall calculations, Ng and Spalding [79], showed that the model also performed fairly well with these flows, provided that an extra term was added to the $kL$ length-scale equation to produce the correct decay of length scale near the wall.

In parallel with this work, Spalding developed his $k$–$W$ model in which he employed an equation for $W \sim k/L^2$ (which is the square of Kolmogorov's frequency $\omega$) as the length-scale-determining equation where the quantity $W$ was interpreted as the time-mean square of the vorticity fluctuations. This work was first reported in Ref. [80] and then in a paper in which he also calculated the concentration fluctuations in a round jet, Spalding [81], a paper which was to serve as a basis for many other papers, especially in the combustion community. An extended account of work on the $k$–$W$ model was provided in an internal report, Spalding [82], which also appeared in a commemorative volume, Spalding [83]. While it may seem strange that Spalding should adopt a different dependent variable from his students, he recognized that this was an area where a range of choices was available and that the advantages or weaknesses of different routes needed to be explored. Indeed, he was supportive of the fact that a group led by one of the lecturers, B.E. Launder, explored the use of an equation for the dissipation rate $\varepsilon \sim k^{3/2}/L$ as the length-scale equation, Hanjalic and Launder [84], Jones and Launder [85].

Spalding made some comparison of various length-scale equations and addressed the question of choice in his 1971 report [82] on the $k$–$W$ model. He stated in this report that "*it cannot yet be said that any model is obviously superior*" – and that the choice could be based upon aesthetic considerations. However, already in 1970 in an internal Imperial College note addressed to his coworkers Spalding analyzed the general length-scale equation for the variable

$$Z = k^m L^n \tag{16}$$

and considered which choice of length-scale variable (i.e., which exponents $m$ and $n$) would best satisfy the requirements for both free and near-wall flows. He came to the conclusion that the variable $\varepsilon$ ($m = 3/2$, $n = -1$), which was then being used by Hanjalic and Jones, satisfied the requirement better than the other length-scale variables investigated at Imperial College at the time. A similar

analysis was published later in Launder and Spalding [74] which established the basis for giving the preference to the $\varepsilon$-equation. The 1970 note states, however, that Kolmogorov's [13] variable $\omega$, which is the frequency of the turbulent fluctuations, could also be a suitable variable, an early finding that is supported by the more recent success of the $k$–$\omega$ model, Wilcox [86], and its 'Shear–Stress Transport' (SST) variant, Menter [87].

In free turbulent shear flows, the models using different length-scale equations produced nearly identical results, as observed in various papers by Spalding; but, of the models investigated at the time at Imperial College, only the $\varepsilon$-equation could dispense with wall-effect corrections (additional terms or variation of the constants). This fact was responsible for Spalding being converted to giving his preference to the $\varepsilon$-equation in the coming years. Among his earlier involvements with the $k$–$\varepsilon$ model were the calculations for the 1972 NASA-Langley conference on free-shear flows [88], to which the Imperial College group contributed calculations of 23 different free-shear flows with a number of turbulence models ranging from the mixing-length hypothesis to a second-moment-closure, those involving a scale-determining equation all using the ε-equation, Launder et al. [88]. These calculations firmly brought out to a largely American audience the superiority and greater generality of the two-equation model over models using an empirical length-scale prescription for free-shear flows. In the years following, Spalding was also involved in calculations of elliptic flows with the $k$–$\varepsilon$ model and this early work was summarized in the paper of Launder and Spalding [74], which for a long time has served as one of the main references for the $k$–$\varepsilon$ model, with numerous citations in the literature.

In the 1980s Spalding returned to his $k$–$W$ model and made the same version applicable to both near-wall and free flows by adding a source term involving the length-scale gradient in the $W$-equation. The model was tested successfully for a variety of flows, Malin and Spalding [64,89], Ilegbusi and Spalding [90]; but by then the $k$–$\varepsilon$ model was so widely accepted that it remained the main model in use. Around the same time Spalding also introduced two-fluid (turbulent/non-turbulent) models involving the calculation of the intermittency. One version was a modified form of $k$–ε model, Malin and Spalding [64], while the other, Ilegbusi and Spalding [65–67], did not use an eddy viscosity but rather a diffusion flux based on the direct calculation of the cross-stream velocity of the two fluids, while reverting, for the length-scale determination, to an empirical prescription. While the ideas were novel, these models did not have any great impact, compared to the advance of the original $k$–$\varepsilon$ model.

Indeed, the $k$–$\varepsilon$ model rapidly became the most widely used two-equation model and, while now superseded at the research level in favour of more general routes to determining the stress–strain inter-linkage, it is still the main workhorse in industrial CFD calculations. While Spalding was neither the developer nor the main advocate of the model, and in fact later expressed doubts about the wisdom of the choice of the $\varepsilon$-equation [91], he played a major and decisive role in developing, promoting and disseminating models of the two-equation eddy-viscosity type which he recognized very early on as the simplest useful level for use within general CFD computer codes since such models required no turbulence quantities to be prescribed within the computation domain. This enabled non-specialists in turbulence modelling to embark on the calculation of turbulent flows for practical configurations over a very wide range of fields.

## 9. Turbulent combustion and chemical reaction

Brian Spalding has made many very significant contributions to the field of turbulent combustion modelling. Indeed, many of the currently prevailing key ideas in combustion modelling were already present in his pioneering developments, including the often-controlling role of mixing at the molecular level, and the multi-scale nature of the problem with the crucial part played by surface phenomena at the flame front. In Spalding's own words, [92]:

> "*Few painters invent new colours: it is their arrangement on the canvas which constitutes novelty.*"

Spalding's most cited contribution to turbulent combustion is perhaps his 1971 paper in the 13th Combustion Symposium [93]. From the experimental observations of turbulent, premixed, confined, bluff-body-stabilized flames available at the time, he reflected on the relative independence of the angle of spread of the flame from the experimental conditions (such as fuel type, equivalence ratio, mean speed of the approaching flow or temperature and pressure levels). From this evidence, he concluded that, for a wide range of flame conditions, the chemical kinetics were indeed subsidiary to aerodynamic processes. In a much earlier, pre-CFD paper published in 1967 [94], Spalding had analyzed the implications of assuming that the fresh mixture was immediately burned as it was entrained into the shear layer (then known as the "entrained-is-burned" model). The assumption provided at the time results in the correct direction; but, from the vantage point afforded by the first CFD calculations years later, it was deemed to be crude. The entrainment-is-burned model was thus replaced in the 1971 paper with the "mixed-is-burned" model, which would be later known as the "eddy-break-up", or EBU, model. The essential feature of EBU is that turbulent burning proceeds at the rate at which large parcels of fresh gas break into smaller ones, thus creating interface area for the molecular processes to act; since it is mainly on this interface area that combustion takes place, at sufficiently-large Damköhler numbers, it was postulated that the rate of combustion can be modelled by recourse to the rate of eddy break-up.

The seminal 1971 paper [92] addressed flames in turbulent shear flows, where, using an equilibrium assumption, the rate of kinetic energy decay can be estimated to be equal to the production. Thus, the reaction rate per unit volume in this mixing-controlled regime was postulated to be:

$$\dot{r}'''_{mix} = C(1-\tau)\rho\left|\frac{\partial u}{\partial y}\right| \tag{17}$$

where $\tau$ is the mixture local reactedness (or reaction progress). An Arrhenius rate was combined with this mixing rate in a harmonic average to cater for situations where chemical kinetics is the rate-controlling process.

The model was further refined in a paper published in 1975 [95] that is one of the first endeavours at the comprehensive, multidimensional modelling of a combustion chamber. The calculation was fully elliptic (as opposed to previous mainly parabolic simulations of laboratory flames); the two-equation $k$–$\varepsilon$ model was used for turbulence; and a four-flux model of radiation was included. Advantage was taken of the $k$ and ε predictions to re-cast the eddy-break-up model into one of its now widespread forms, viz.

$$\dot{r}'''_{mix} = Cg^{1/2}(\rho\varepsilon/k) \tag{18}$$

where $g$ is the scalar (mixture-fraction) variance [81].

The eddy-break-up model, as described above and used for several decades (with minor, non-fundamental variants) by many researchers was largely regarded by Spalding as a first, crude attempt [93,95] to account for the often-controlling influence of flame aerodynamics on the combustion rate, and of the relevance of the micro-scale phenomena of interface-surface creation and of molecular mixing across this interface. The original EBU model

was therefore much refined in subsequent research by Spalding and co-workers. Thus, in [96,97] he outlined the ideas for a "slide-and-stretch" model of turbulent combustion, in which "coherent bodies of gas are squeezed and stretched as they travel through the flame". The idea was further elaborated in [98], and was subsequently given its own character as the ESCIMO model.

ESCIMO stands for *E*ngulfment, *S*tretching, *C*oherence, *I*nter-diffusion and *M*oving *O*bserver, i.e., the main constituents of the model. Spalding, drawing from the ideas of many previous authors, formulated a model [100] that can be regarded as the first multi-scale interpretation of turbulent combustion suitable for embodiment in a CFD code. Chemical reaction was, as for EBU, assumed to take place in the interface area separating the reactants (in diffusion flames) or reactants and products (in premixed flames). The interface area was arranged in what were equivalently termed "folds", "parcels", "sandwiches", or "layers" (Fig. 2); these are formed in the main shear regions of the flow; they stretch as they are convected; and then 'die' when they are re-engulfed by other eddies. The task of ESCIMO was therefore twofold: first, to calculate the statistics of the folds (i.e., the local distribution of their sizes, or widths), which was called the "demographical part" [100]; and, second, to compute the (one-dimensional) property distribution within each fold (which was termed the "biographical part"). The first is an Eulerian point of view; the second is Lagrangian, because the transient, one-dimensional profiles depend (barring simplifications) on the fold history as it moves through the flow (this is the Moving Observer part of the model name). Also the first describes the flow in the macro-scales, where convection and stretching occur, while the second focuses on the microscales, where molecular diffusion and chemical reaction take place. The ESCIMO model was applied by Spalding and co-workers to several canonical configurations, such as stirred reactors, baffle flames and free jets [100,101], for which analytical solutions for the fold populations could be calculated with suitable simplifying assumptions. It was later successfully applied to turbulent, non-premixed hydrogen–air flames [100].

The uptake of ESCIMO by the scientific community at large was scanty, despite the fact that it embodied, in a framework which rendered the problem solvable with the late 1970s computers, the key concepts later found in widely-accepted models. Thus, flamelet models of non-premixed combustion make use of the same notion of a distribution of thin reaction layers, which are parameterized using not a length scale (the fold width) but the inverse of a time-scale (the dissipation rate). The time-dependence of the biographical part of the fold (e.g., the species one-dimensional profile within the layer, Fig. 2), is dispensed with in the so-called steady-state flamelets. This is calculated locally, irrespective of the parcel (or flamelet) history. The more recent, and independently derived, linear-eddy model (LEM) of Kerstein [102] remarkably shows some common modelling principles with ESCIMO. Notably, LEM resorts also to a one-dimensional calculation, embedded in the three-dimensional one, to resolve the coupling between mixing and chemical reaction in the small scales that cannot be resolved by the 3D mesh. Unlike Spalding's ESCIMO, the small scales are calculated in an Eulerian framework; and the effect of turbulent mixing is simulated through stochastic stirring of the one-dimensional field, rather than by using a local "eddy distribution".

The development of Eulerian multiphase methods such as IPSA [60,103], discussed above, opened up new opportunities to add physical realism to turbulent combustion modelling. Spalding soon recognized that the flame front, where burned (burning) and unburned matter intermingle as in a "land-and-lagoons landscape" [68], and could be modelled as a two-phase flow, with one phase representing the burning fluid and the other the unburned one. Combustion is therefore regarded in this framework primarily as an interface phenomenon taking place on the parcel boundary, and triggered by the entrainment of fresh fluid into the burning one. The combustion rate was primarily governed by this entrainment rate, which required modelling. The models for entrainment often involve the fragment surface area per unit volume, which is the inverse of a length scale and can be interpreted as a characteristic fragment size; several algebraic and transport models have been suggested for this fragment size. Kinetic control of combustion is also provided within the burning fluid. It is interesting to note that a similar concept underlies the single-fluid eddy-dissipation concept of Magnussen [104], where the "fluids" (using Spalding's term) are the "surroundings" or mean mixture and the

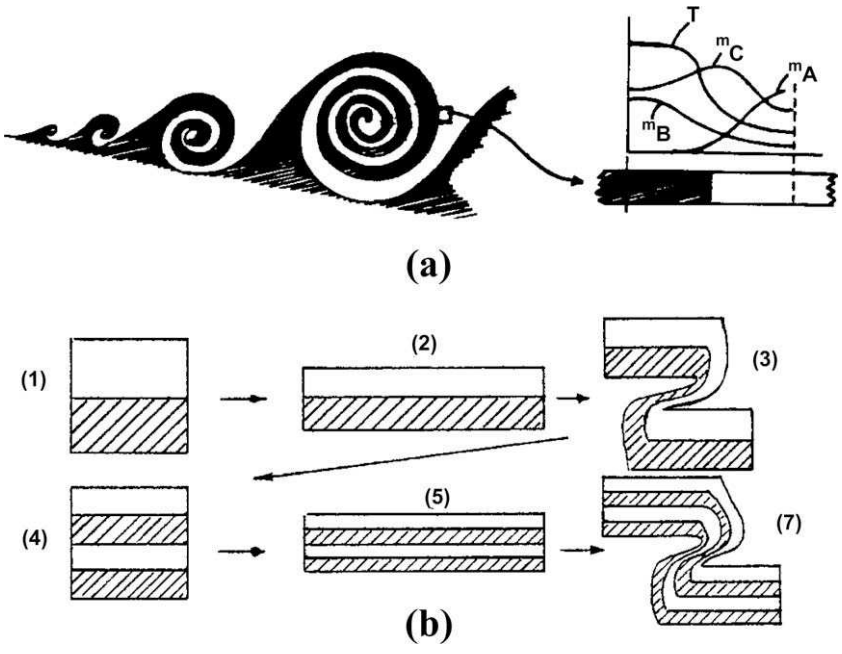


**Fig. 2.** The ESCIMO model: (a) the "folds", from [99]; (b) "sliding and stretching". From Ref. [92], with permission.

"fine structure"; in the latter, the reactants are mixed at the molecular level. Spalding's interphase-transfer rate is the rate of creation of fine structure in the eddy-dissipation model.

Because of its true two-phase character, Spalding's two-fluid model provided the benefit of allowing for two different local densities (for the fresh and burning fluids, respectively). Fluid fragments with different densities react differently to a common pressure gradient, thus originating a "non-gradient" (and, sometimes, "counter-gradient") diffusion, which conventional models cannot reproduce, but two-fluid ones can [69,70].

The "unburned-burning" (or colder–hotter) model of turbulent combustion is just an instance of the new class of two-fluid turbulence models pursued by Spalding. While "heavier–lighter" models, such as the combustion one outlined above, allowed for a representation of the "sifting" phenomenon (i.e., fragments of fluid with a given density moving through fragments with another), in other models a property other than density was selected as a fluid-distinguishing property, as indicated in the turbulence modelling section above.

The latest member in this lineage of increasingly sophisticated models which build upon similar principles are the multi-fluid models (MFMs) of combustion and chemical reaction [105,106]. MFMs are often introduced by Spalding as an evolution of the eddy-break model [107]. While in the EBU model only two thermochemical states are permitted (burned and unburned), in MFMs an arbitrary number of intermediate states are allowed by defining population defining attributes (PDAs), such as mixture fraction and/or reactedness. These PDAs are discretized, and several fluids are allowed to co-exist in the domain, each characterized by a set of values for the PDAs. The multifluid model solves conservation equations for the local mass fraction of each fluid. In the turbulent flow, fragments of these fluids with different compositions collide (the collision among fragments being an idea originally behind the theories on turbulence of Reynolds and Prandtl); and, after some contact time, separate, thus leading to a certain fraction of intermediate fluids at the interface, which Spalding terms "the offspring". The population distribution is in this way changed. The theory allows also for "continuously-varying attributes" in the fluids, i.e., properties which are not discretised.

The intuitively developed MFMs share many analogies with the mathematically derived probability density function (PDF) equation solved with a Monte Carlo method [108,109]. Fluid fragments are akin to fluid particles; however, while the defining properties of the former are discretised as population defining attributes, the properties of the Monte Carlo particles are allowed to vary continuously. In both approaches, micro-mixing is modelled when two fluid fragments collide: in the Monte Carlo method, the so-called molecular mixing models, which frequently address mixing as a particle–particle interaction are used; in MFMs, mixing is represented through the rate of mass transfer between the colliding fluid fragments as they enter in contact with each other, resulting in the "offspring". In MFMs, the PDF can be reconstructed from the mass fraction of the fluid population.

CFD has been applied to the prediction of the performance of combustion processes since the 1960s, and Spalding and the Imperial College team pioneered the use of the technology for combustion calculations. First, Patankar and Spalding [42] devised the milestone GENMIX CFD code for the calculation of parabolic flows, and during 1969 Spalding incorporated combustion into GENMIX, [45,50], which could simulate laminar and turbulent flame jets, and was later used for the prediction of laminar flame propagation by Spalding and Stephenson [110]. Spalding proposed a CFD model for Diesel Engines in 1969 [111,112], but even as early as 1967, Spalding had employed the simple chemical reacting system (SCRS) concept into a CFD code for the simulation of turbulent diffusion flames in furnaces, Pun and Spalding [113]. An underlying feature of the model is that the combustion process is represented by a global, one-step, infinitely fast chemical reaction in which fuel and oxidant react to form products at stoichometric proportions. The intermediate species are ignored, and the mass fractions of the reactants, product, and inert species are expressed as fixed algebraic relationships in terms of a conserved scalar variable called the mixture fraction. This approach was to become the basis of all CFD modelling of furnaces and combustors for some time to come, and it was soon extended by Spalding and co-workers to allow fuel and oxidant to co-exist at the same location, although at different times, by the use of a presumed probability density function (pdf) and the solution of a transport equation for the variance of the mixture fraction. Thus, the presumed-pdf model probably started in CFD with Spalding's "two-spike" double-delta-function presumption [114], and subsequently, Lockwood and Naguib [115] made the "clipped-Gaussian" presumption; and they were followed by many others, including Kent and Bilger [116]. The third type of combustion model pioneered by Spalding's Imperial College team was to employ the SCRS with a finite reaction rate represented by the minimum of the Arrhenius and Spalding's eddy-break-up model in the transport equation for the fuel mass fraction. These three combustion models are documented, and applied to a number of furnace arrangements in a paper by Khalil et al. [95], which reports on the modelling work performed under contract to the Atomic Energy Research Establishment (AERE), Harwell (UK). This paper dealt with two-dimensional flows, however three-dimensional furnace flows had, in fact, already been simulated by Patankar and Spalding [117,118], and applications to three-dimensional gas–turbine combustors were soon to be published by Serag-Eldin [119].

## 10. Partially parabolic and complex flows

One of the early applications of the three-dimensional parabolic procedure was to ducts with curvature. In 1972, immediately after the publication of the parabolic calculation procedure, Pratap[5] [120], working under the supervision of Spalding, attempted the computation of flow and heat transfer in helically coiled pipes. This work consisted of the study of both the developing and fully developed regions, the fully developed being the spatially asymptotic state. Flow in coiled pipes is of importance in a variety of applications such as heat exchangers, river bends, curved arteries, pipe elbows, etc. When fluid flows through a curved duct the curvature of the duct induces secondary flows which are directed to the outside in the central region and towards the inside in the near-wall region. These secondary flows are referred to as Dean vortices [121,122]. In the developing region, the streamwise flow evolves from a parabolic profile to a distorted profile with a peak on the outside region. This is a result of the momentum transfer from the inner region to the outer region of the bend.

Prior to 1972, there had been no computations of the developing region of the helical coil. Pratap et al. [123] published the first paper on laminar developing flow in a curved pipe. In this paper, the developing region was solved by the parabolic calculation procedure and the streamwise profiles were successfully compared with the data of Austin [124]. Subsequently, the heat transfer enhancement was also compared with experimental data of Mori and Nakayama [125] and Dravid et al. [126] for Pr = 4.0 and 0.71, respectively. This paper revealed the ability of the parabolic duct flow procedure to predict industrially relevant complex flows. This procedure was next extended from laminar flow to turbulent flow. Here, the momentum and continuity equations for a curvilinear coordinate system were augmented with the $k$–$\varepsilon$ turbulence model [127]. The

[5] V.S. Pratap is currently known as S.P. Vanka.

above two works considered large radius ratios. However, when the duct curvature is large the parabolic assumption can break down. Spalding proposed a new procedure, called the 'semi-elliptic', or 'partially parabolic' procedure, which accounted for such cross-stream pressure variations in accelerating the streamwise flow. This idea was followed up by Pratap and Spalding [128] who demonstrated the possibility of capturing such effects. This procedure was applied to the flow in a duct with strong curvature, and experimental data taken by Pratap [129] were used for comparison.

Flows in ducts rotating about an axis perpendicular to the duct axis present another situation with body forces on the fluid. Majumdar et al. [130] applied the three-dimensional parabolic calculation procedure to solve the governing three-dimensional flow equations in their parabolic form. The momentum equations contain extra terms due to the centrifugal and Coriolis forces. In a subsequent study, Majumdar and Spalding [131] applied the partially parabolic procedure to flow in rotating ducts. Agreement with data was generally good; however certain discrepancies were observed. This algorithm recognizes that the three-dimensional scalar pressure field is indeed elliptic and that there is fluid recirculation in the cross-plane of the flow, which demands the allocation of scarce computer memory to pressure and velocity components, but since there is no downstream to upstream flow in the main flow direction, then only the pressure need be stored in memory as the flow then essentially acts parabolically. Pollard and Spalding [132] took this idea and developed a partially elliptic method.

Majumdar et al. [133] studied the local and mean heat-transfer characteristics for air flowing turbulently in the fully developed region of a circular and of a square duct rotating around a horizontal axis parallel to the duct axis. Results showed that the heat transfer was increased by rotation. The results were compared with experimental data with good agreement. A prior study by Majumdar [134] also considered radial diffusers that were rotating about a perpendicular axis.

The development of the partially parabolic algorithm was a testament to Spalding's grasp of the physics of fluid mechanics, and of transport phenomena in general. The above works on flows with body forces – duct flows influenced by rotation and curvature – were path-breaking. The newly developed partially parabolic (as well as the parabolic) procedures were successfully applied. These led to a new set of computational procedures to predict complex three-dimensional flows which, by 1975, were being considered in the Heat Transfer Section at Imperial College (a 'complex flow' then being defined as one with externally applied rates of strain or in which two or more basic turbulent flows interact [135], as opposed to 'basic flows': jets, wakes, channels, boundary layers). One element of the research focus during this period was to establish the competency to predict three-dimensional turbulent flows using the turbulence models, discussed elsewhere in this paper. In many cases, experimental data were also required, and if the equipment existed in other parts of the world, students were sent there. A review of the 75 or so papers that emerged from the group during the period of 1970–1980 reflect the vast number of topics that engaged Spalding, for example: free and forced turbulent convection, Abdelmeguid and Spalding [136]; flow over and around various shapes and obstacles, Caretto et al. [137] combustion, Serageldin and Spalding [138]; low-Prandtl number heat transfer, El-Hadidy et al. [139], flows in T-junctions, Pollard [140]; two-phase flow, Majumdar et al. [141]. A significant feature of many of these investigations was the combination of the development of computational methods and models that better captured the main features of the physics of the phenomena under study.

High performance computers are widely prevalent nowadays; however, in those days, computing devices were quite modest in terms of both memory and speed. Thus, what would today fit into a small handheld device, then required a huge infrastructure and large numbers of support personnel. Restrictions on memory size and data-storage did not always permit the desire to solve the Navier–Stokes equations for large-scale problems to be satisfied. Thus, innovative algorithm development was always an integral part of the CFD community activities. In the early to mid 1970s, two-dimensional flows were being computed, but on what today seem like very small numbers of control volumes. With the addition of new hardware with more memory and storage, and the development of floating point operations, the idea of solving equations in three-dimensional space and even time could be contemplated; however, with that, there was the need to invent even more elegant algorithms.

## 11. Heat exchangers

Patankar and Spalding [142] first proposed to perform 3D calculations for fluid flow and heat transfer in shell-and-tube heat exchangers by means of a porous medium or 'distributed resistance' analogy. This was essentially a very early example of a multi-scale analysis, where detailed computations around the baffles of the heat exchanger were performed but drag and heat transfer were 'modelled' based on prescribed volumetric friction and heat transfer factors. These factors were to be obtained either analytically, or from detailed fine-scale numerical calculations, LeFeuvre [143], Beale and Spalding [144], or from correlations of experimental data. This approach was quite different from conventional heat exchanger design approaches based on 'presumed flow' methods, such as the Delaware method [145]. As previously mentioned, the partial elimination algorithm (PEA) proved most beneficial in this context, since in later applications (see below) the volume-averaged equations for shell-side, and tube-side fluids closely mimicked those for two-phase flow and heat transfer. The Patankar–Spalding approach was subsequently adopted and refined by a number of other researchers. A complete discussion of Spalding's philosophical approach to heat exchanger analysis may be found in his articles in the Heat Exchanger Design Handbook [146]. This subject has remained one of enduring interest and Spalding continues to lecture on the subject to this day [147].

## 12. Stress analysis

What numerical method is typically used by engineers to calculate stresses and strains in solid objects? The usual answer is the "Finite Element Method" (FEM), which is routinely applied to the simulation of structural analysis problems, and forms the basis for many computer codes. There are, however, numerous multi-physics problems, where solid stresses must be computed at the same time as, say, turbulent fluid flow with heat and mass transfer, chemical reactions and so forth. Such fluid–solid interaction (FSI) problems are of much scientific interest and practical necessity. Some examples include thermal and centrifugal stresses in a rotating turbine, pressure wave propagation in fluid flow in an elastic tube such as blood-flow in human arteries, or flow in a printer-head chamber containing a piezoelectric membrane, to name but a few. In these and other cases, the choice of methodology is less clear since FEM algorithms are arguably not as sophisticated for simulation of coupled systems of hydrodynamic equations, compared to the finite-volume method (FVM), which is well developed and currently employed in almost all major CFD codes. Moreover, such CFD codes already contain numerous sub-component models for physical phenomena (turbulence, radiation, chemical reactions, multi-phase flow, etc.) which are necessary constituents for modelling complex FSI problems.

Spalding was among the first to propose that the FVM may readily be adapted to obtain solutions for elasticity problems

and, to suggest that it is probably simpler to develop the equations in a FVM-based code, than to port the large set of existing physical fluid mechanics and heat transfer models from established FVM based CFD codes over to FEM-based codes. Beale and Elias [148,149] showed how the FVM code PHOENICS could be applied to stress analysis problems using the analogy between the stream and stress functions in creeping-fluid-flow and solid mechanics. That approach was notionally similar to the $\psi$–$\omega$ methodology of Runchal et al. [43], and was thus limited to two-dimensional plane strain/stress problems. Spalding subsequently considered a displacement, rather than a force analogy which has the major advantage of being quite general in three dimensions.

The governing equations for linear thermo-elasticity are based on the equation of equilibrium, which combined with the generalized Hooke's law and the strain–displacement relations, result in Navier's displacement equations. Spalding originally considered the displacement equations in the following form,

$$G \text{ div grad } \mathbf{u} + \mathbf{f} - \text{grad } p = \mathbf{0} \tag{19}$$

where

$$p = -(\lambda + G)D + H(T - T_0) \tag{20}$$

where $\boldsymbol{u}$ is displacement, and $\boldsymbol{f}$ is a body-force. The 'pressure' $p$ is thus proportional to the cubical dilatation, $D = \text{div}\mathbf{u}$, where $\lambda$ and $G$ and are Lamé constants, and $H$ is proportional to the coefficient of thermal expansion. Eq. (19) strongly resembles the (Stokes) momentum equation for creeping flow. Thus, Spalding [150] first proposed in 1993 the FVM solution of FSI problems, based on this analogy between the equations for displacement (solids) and velocity (fluids), with the following modification to the usual FVM: in fluid regions $\boldsymbol{u} = (u, v, w)$ represents velocity whereas in solid regions, it represents displacement. In the latter, the convection terms are set to zero. The linear relation between pressure $p$, dilatation $D$ and $T$, Eq. (20), is introduced by the inclusion of a pressure and temperature dependent 'mass-source' term. Strains and stresses may readily be computed from the displacements. Later, Spalding [151] replaced the pressure/dilatation term in Eq. (19) with anisotropic exchange coefficients, $\Gamma$, for the solid-phase-diffusion terms. He also noted that other forms of the governing equations, for example based on rotation (the stress-equation counterpart to vorticity) are possible, and may ultimately prove superior to displacements. For the solution algorithm it is possible to use the well-known SIMPLE algorithm, but in [151] Spalding speculated that coupled schemes such as the SIVA algorithm [52] may be more effective in this context. Combined solid-thermal fluids problems, for example, in porous media, should prove readily amenable to this class of analysis in the future. The unification of stresses and strains into the general framework of fluid flow and heat transfer with chemical reactions and turbulence, is another logical step forward in the development of a general-purpose engineering methodology founded upon physical reasoning.

## 13. Concentration Heat and Momentum Ltd.

There can be little doubt that Spalding and his associates pioneered the commercial CFD industry by founding the company, originally known as Combustion Heat and Momentum Ltd. (CHAM) in 1969. The company, which became Concentration Heat and Momentum Ltd. in 1974, provided commercial CFD services based on the pioneering technology that had emerged from Spalding's research group at Imperial College. While the activities of CHAM and the genesis of the CFD code PHOENICS (see below) are irrevocably intertwined, well before the advent of PHOENICS, CHAM was essentially the world's only commercial CFD company, and remained so until the early 1980s when Creare Inc. began marketing the FLUENT code, the early origins of which can be traced to Swithenbank et al. [152]; see also Runchal [153]. Between 1974 and 1980, CHAM developed many application-specific CFD computer codes for industrial clients across a wide range of industrial sectors, including the aerospace, automotive, defence, chemical, environmental, fire and safety, marine, manufacturing and process, nuclear-power, and fossil-fuel power industries. These CFD codes (some of which found their way into the public domain) also provided the means for CHAM to undertake CFD consultancy contracts aimed at solving practical problems for industry. CHAM's clients were for the most part, large engineering companies in the UK, Europe, and the USA. During this period CHAM scored numerous 'firsts', under Spalding's direction and supervision. For example, it created the first CFD code for the steam generators of the nuclear industry: for this, CHAM had to devise CFD programs which could simulate the separate flows of steam and water within the same space. As another example, CHAM produced the first Electrolytic SmelTER (ESTER) CFD code, for the aluminium-production industry, to simulate multi-anode electrolytic smelters of the Hall-cell type, in which electromagnetic effects and gravity waves on the molten-metal/electrolyte interface can interact to limit the performance of the equipment. Later on, ESTER was superseded by a PHOENICS-based product, Rosten [154], that was also used extensively by the industry [155–157]. Coal- and gas-fired furnaces, heat-exchangers, diesel and petrol (gasoline) engines, power condensers, steam generators, and natural-draught cooling towers were all among the equipment items for which CHAM produced the first CFD packages.

During the 1970s the partially parabolic method, described earlier, provided CHAM with a more practical route than fully elliptic codes for some 3D industrial applications. For example, the partially-parabolic CFD code FLASH was employed to compute 3D flow around ship and submarine hulls using a curvilinear coordinate system. This work was largely funded by Ishikawa-Harima Heavy Industries (IHI) (Japan), National Maritime Institute (NMI) (Teddington), and Admiralty Experimental Works (AEW) (Haslar), and resulted in a substantial number of publications by Spalding and co-workers, e.g., Abdelmeguid et al. [158] and Markatos et al. [159]. As computer technology became more powerful, FLASH was superseded by an in-house elliptic CFD code, and then ultimately by a PHOENICS-based CFD model, with a general non-orthogonal body-fitted coordinate system, Malin et al. [160]. The partially parabolic concept also proved useful in turbomachinery applications, and in 1976 the SEMFT partially-parabolic CFD code was developed by Singhal and Spalding [161] for predicting 2D steady, turbulent flow in turbomachinery cascades. This code, supplied to Sulzer Brothers in 1977, was capable of handling incompressible, subsonic, supersonic, or transonic flows. The CATHY3 code was another partially parabolic turbomachinery code that was supplied to a number of companies, including the Westinghouse Electric Corporation in 1978. A curvilinear coordinate system was employed for the prediction of steady, 3D turbulent flow in rotating turbomachine passages. The code was derived from earlier work by Pratap and Spalding [128] and Majumdar and Spalding [162]. It was replaced in 1979 by a fully elliptic code of the same name, Malin et al. [163]. This elliptic CFD code included a cavitation model, and the software was supplied to NASA Marshall for the prediction of steady, 3D turbulent flow in centrifugal impellers.

As was mentioned earlier, Patankar and Spalding [142] pioneered the use of the distributed-resistance concept in CFD modelling of 3D flow and heat transfer in a shell-and-tube heat exchanger. This approach has been used extensively by CHAM since the early 1970s for conducting CFD simulations of heat-exchanger, steam-generator, and condenser applications in the defence, marine, nuclear, and power industries. These applications were funded by numerous companies including Combustion

Engineering (USA), Rolls Royce (UK), National Nuclear Corporation (UK), Electrical Power Research Institute (USA), European Atomic Energy Community (Italy), Northern Engineering Industries Parsons (UK), General Electric Company (UK), and Vattenfall (Sweden). The publications resulting from these and other studies by Spalding and co-workers were numerous, see, for example, Singhal et al. [164,165], Al-Sanea et al. [166], Jureindini et al. [167], and Malin [168]. Some applications included the simulation of two-phase flow by means of homogeneous, algebraic-slip or two-fluid modelling via IPSA. Eventually PHOENICS became the vehicle for all such computations at CHAM, but notable pre-PHOENICS CFD codes developed by Spalding and other CHAM personnel were ATHOS, CALIPSOS, FOCS, LOBSTER, STELLA, and URSULA.

The origin of many industrial multi-phase computations can be traced to GALA [61,62] and IPSA [60,61], both devised by Spalding in the mid seventies. These were described earlier in the manuscript, but it should be mentioned here that Spalding's remarkable paper [61] also describes different interface-tracking techniques as alternatives to using GALA for the simulation free-surface flows. One method involves tracking particles, while the other involves the solution of a conservation equation for the liquid height. Interface tracking techniques were employed successfully both by CHAM as well as the group at Imperial College in the late 1970s and early 1980s, see, for example, Maxwell [169], Awn [170], and Castrejon and Andrews [171]. IPSA has made a tremendous impact on the numerical computation of industrial multi-phase flows. It formed the basis of the bulk of the two-phase flow simulations made by CHAM and its clients with PHOENICS and earlier CHAM codes, Moult et al. [172], Baghdadi et al. [173], Markatos et al. [174,175], Marchand et al. [176], Al-Sanea et al. [177], Boisson and Malin [178]. Inevitably, the method later found its way into competing commercial CFD products.

Spalding was content to employ the algebraic slip model for many suitable multi-phase-flow applications. This model was in use at CHAM during the late 1970s for steam-generator applications, Singhal et al. [179,180], but its use became much more widespread during the 1980s for use in the chemical and materials processing industries. Several variants of the model were in use during this time, mostly restricted to considerations of gravitational and/or centrifugal force fields, for example: Pericleous and Drake [181] (particulate separation in cyclones); Tacke and Ludwig [182] (inclusion separation in tundishes); Pericleous and Patel [183] (solid suspensions in stirred tank reactors). Eventually, Spalding proposed a more general formulation that employed GALA for the satisfaction of volumetric continuity. The method was implemented in PHOENICS in 1992. In more recent times, multi-phase capabilities using algebraic slip modelling began to appear in other general-purpose CFD software.

During the mid 1970s to early 1980s another novel application-area was the prediction of fire and smoke movement in buildings. At that time, the Fire Research Station, Borehamwood UK (FRS) funded CHAM's pioneering work in the development and application of the 2D and 3D elliptic MOSIE CFD codes, Markatos et al. [184]. These special-purpose fire-and-smoke simulation codes were superseded by a PHOENICS-based model, which was subsequently used by the FRS and later by the Building Research Establishment (BRE), to create the well-known CFD fire-simulation code JASMINE, Markatos & Cox [185], Kumar et al. [186], which makes use of an early version of the PHOENICS code as its CFD engine. In this way, Spalding's contribution can be seen as providing FRS and BRE with a basic CFD capability from which they were able to develop and validate the CFD technology embodied in JASMINE to such an extent that CFD now forms an accepted component of fire safety engineering.

In the early years at CHAM, combustion modelling formed a significant part of the business, and by 1973 the company had created for the Rocket Propulsion Establishment (Westcott, UK) a very advanced elliptic CFD combustion code called BAFL, see Tatchell and Spalding [187] and Jensen et al. [188], for predicting flow, combustion and heat transfer in the region immediately downstream of a rocket moving at supersonic or subsonic speeds. BAFL was ahead of its time, and it incorporated a number of sophisticated mathematical models which enabled it to handle compressible, turbulent, recirculating flow with two-way chemical reactions between gaseous species, fluctuations of temperature and concentration, radiative heat transfer in particular wave-length bands (Lockwood and Spalding [46]), and reaction with particulate species in distinct size ranges (Spalding [189]). Indeed, some of the first CFD codes sold by CHAM to gas–turbine manufacturers were specifically for combustor simulation. Several of those combustor codes remained in use for well over a decade, having of course also been significantly further developed by their users; and at least one of them entered the public domain by way of the US Army, enabling competing CFD-code vendors to start business; which they did with alacrity. In 1976, CHAM supplied the NASA Lewis Research Centre with a combustion CFD code using a chemical equilibrium model for characterising hydrocarbon reactions, and a chemical kinetics model for predicting the oxides of nitrogen, Elghobashi et al. [190]. This was perhaps the first CFD model for predicting pollutant formation. Another notable CHAM combustion code of the 1970s was CORA3, which was delivered to a number of industrial clients. This CFD combustion code, among others, made use of Spalding's 'eddy-break-up' [93,191] and 'presumed-pdf' methods [81,191], which took account of turbulent fluctuations. The impact of Spalding's work on CFD in the power generation industry was mentioned by Fiveland, see Hanna [192], who started CFD research work in the boiler manufacturing industry during the 1970s at Babcock and Wilcox in the USA:

> "*At the time I was aware of Professor Spalding's pioneering CFD work in the UK, and we saw value in using this "new" CFD technology to improve our boiler and burner designs.*"

Computers during the 1970s had small memories and slow execution times, and so ingenious programming was needed to enable industrial problems to be solved. Moreover, there was much skepticism in some circles as to whether computer simulation of complex turbulent and multi-phase flows would ever be of any practical use. Some time in 1978, Spalding conceived the idea of a single CFD code capable of handling all fluid-flow processes. Consequently, CHAM abandoned the policy of developing individual application-specific CFD codes, and during late 1978 the company began creating the world's first general-purpose CFD code: PHOENICS.

## 14. The PHOENICS code

Many scientists and engineers distinguish themselves by writing a monograph on their field of expertise, at some point in their careers. Spalding however devoted his time and energy instead to a practical piece of CFD software, which in turn helped spawn a whole industry-field, and created jobs and wealth, where none previously existed. CFD as a sub-set of computer aided engineering can thus be directly traced to the developments of the *P*arabolic, *H*yperbolic *O*r *E*lliptic *N*umerical *I*ntegration *C*ode *S*eries, PHOENICS [51,193–195].

PHOENICS was launched commercially in 1981 as a FORTRAN-input program and later, in 1984, as an interactive-input CFD code. Here for the first time a single code was to be used for all thermo-fluids problems. This represented a major philosophical change. Indeed, at the time, there was substantial resistance to the idea that a general-purpose CFD code was even possible. Credit for PHOENICS

is due also to a number of other people, especially H.I. Rosten, and it would be remiss not to mention the significant and ongoing contributions made since the code's inception by J.C. Ludwig. However, PHOENICS was essentially Spalding's brainchild, and remains the subject of his attention to the present day. PHOENICS represented a paradigm shift in the advance of CFD; engineers were now able to apply the algorithms and closure assumptions previously developed at Imperial College and elsewhere to a whole host of real-world industrial problems. Once this step was reached CFD advanced irreversibly beyond the ivory tower of academia and into the real world of engineering products and processes. The requirement to provide a working software product to a client led to a new level of professionalism, in terms of software design, memory management/optimization, portability, documentation, and training, not typically found in a university environment. Because of the general-purpose nature of the code, CFD advanced beyond thermo-fluids to a whole range of multi-physics problems, for example, chemical-vapour deposition to give one example.

In the early 1980s, PHOENICS was the only general-purpose CFD code available, and represented an embodiment of many of the scientific principles previously published by Spalding's group, many of which were meticulously reproduced in a case-library for execution by the user. The concept of writing a single- and multi-phase code, for laminar or turbulent flow, with complex chemical kinetics, heat and mass transfer (including thermal radiation) and variable properties was quite unique. The code was designed with a central core known as 'EARTH'. This contained all established utilities which were hard-coded and to which the user did not have access (in order to avoid damage by the inexperienced and thus to facilitate maintenance and support). Open source components were also provided wherein physical models such as turbulence closures, wall functions, and solution algorithms were coded and could be inspected, altered or replaced by the user. 'Hooks' (threads) were provided at different points in the software for users to attach their own coding, thus allowing the extension of the code capabilities and enabling it to be used for many problems for which it was not specifically designed. This 'open-source' concept, which was pioneered in 1981, was later adopted by some other CFD-code vendors. PHOENICS was firmly based on the finite-volume method. At the heart of code was the single-phase SIMPLEST algorithm [58], a variant of SIMPLE [55,137]. Multiphase flows were accommodated using IPSA [60] (Eulerian) and GENTRA (Lagrangian). Users could select from a number of linear equation 'solvers' such as point-by-point, slab and whole-field (or indeed provide their own), and control relaxation using inertial or linear methodologies on a per-variable basis. Originally a staggered velocity scheme [53] was employed, although later collocated schemes [196] were added as an option both in rectilinear and body-fitted coordinates. Boundary conditions and the source terms themselves were coded as linear source terms, $S = GC(V - \varphi_P)$ in Eq. (11), where $G$ is a geometric factor, $C$ is a source-term 'coefficient' and $V$ is a source term 'value', over which the user could exert substantial control; thus they were programmable. The code was based on a segregated scheme with a number of 'iterations' being performed for each field-variable, together with multiple 'sweeps' over the entire computational field, until convergence was reached and the solver stopped. Spot-values and residuals were originally printed and, in later versions of the code, plotted dynamically by the graphical user interface (GUI), to provide the user with a measure of confidence in the results.

In early versions of PHOENICS, users were provided the opportunity to tailor the code to their needs using FORTRAN either in the pre-processor, 'SATELLITE', or at run-time, in 'GROUND'. Through GROUND, the user could in fact access all EARTH variables and arrays which were stored in a single '*F*-array' by means of functions and sub-routines which performed a variety of operations. The nature of the code allowed for extensive programmability, so that users could if they wished, completely by-pass all the default solvers and so forth, in favour of their own utilities. It is important to emphasise the enormous number of academic and industrial CFD computations that have been based on the PHOENICS code. The proceedings of the First International PHOENICS Users Conference in 1985 [197] reveals that from the beginning there were a large number of applications of PHOENICS across a very wide range of industries. Subsequent User Conferences, held biennially to date, together with publications in the PHOENICS Journal of Computational Fluid Dynamics, and in the open literature, served to enlarge the number of industrial applications to truly immense proportions. Numerous PhD theses were conducted by Spalding's students at the Computational Fluid Dynamics Unit at Imperial College [198–215] and elsewhere, based on PHOENICS. While nowadays the notion of post-graduate students utilizing a commercial code in their research work is scarcely controversial, at the time it was quite novel.

Some of the code developments included: body-fitted grids (1983); biological flows – bladder, lung, etc. (1987); programmable input language and conjugate heat transfer (1989); expert-based system to improve convergence (1991); solid stresses/strains (1992); parallel implementation (1993); and fine-grid embedding (1997). Later, new programming features were introduced which allowed users to create their own physical models without the need to resort to FORTRAN. As the user-base grew, so did the library of cases. Over the years, innumerable developments by users, both industrial and academic were adopted into the code. In addition, special versions of PHOENICS were developed for a wide range of applications: electrolytic smelters, chemical-vapour deposition, electronic cooling, blast furnaces, cooling towers, external aerodynamics. Special-purpose PHOENICS User Groups were established by CHAM.

PHOENICS was the world's first general-purpose CFD code; and by the time of its release in 1981, the underlying scientific principles had been extensively published. Therefore, once CHAM showed that a general-purpose CFD code could be created and marketed profitably, competitors soon followed the lead. The practices and principles embodied in PHOENICS have been much imitated; and there are now numerous such CFD packages in the market offered by competing vendors. The lineage of most of these codes can be traced back either to CHAM itself or to the Imperial College team from which CHAM emerged, and the influence of CHAM and PHOENICS was sometimes affected by staff movement. Certainly, it can be argued that CHAM's innovation in creating and marketing PHOENICS founded a worldwide industry which is based on the selling of CFD software and services, which although no firm figures are available, now has an annual turnover in excess of six figures.

Within a few years of the first release of PHOENICS, Spalding initiated work at CHAM on the creation and marketing of PHOENICS-based, special-purpose products (SPPs) that employed application-specific GUIs. The first of these was ESTER, which was developed specifically for the aluminium industry. Other SPPs quickly followed in the late 1980s and early1990s, for example, HOTBOX (for electronics cooling), FLAIR (for heating, ventilation and fire and smoke movement in buildings), TACT (for cooling towers), PHOENICS-VWT (for motorsport vehicle aerodynamics) and PHOENICS-CVD (for chemical-vapour-deposition). Spalding argued for the application of CFD to CVD reactors as early as 1979 [216], including a proposal to use embedded fine-grids to resolve more accurately the fine structure of the fluid flow and deposition process in the vicinity of the wafer.

PHOENICS-CVD, Heritage [217], remains the most technically-advanced of the SPPs, being able to simulate the behaviour of a wide range of CVD reactors by modelling fluid flow and heat

transfer in a multi-component gas, including both gas-phase (homogeneous) and surface (heterogeneous) chemical reactions, thermal radiation and plasma effects. During the 1980s and 1990s, PHOENICS was heavily used by CHAM and other organizations for metallurgical- and materials-processing applications. Such applications are often challenging and can involve combinations of fluid-flow, heat and mass transfer, phase change, electromagnetics, free-surface flow, multiple phases, and chemistry. The successful use of PHOENICS-ESTER by the aluminium industry has already been mentioned. In addition Alcan International collaborated with CHAM to use IPSA in PHOENICS for simulating the mixing and solidification of submerged liquid metal jets, see Enright et al. [218]. CHAM also used IPSA to create PHOENICS-based CFD models for the NASA Lewis Research Centre to simulate solid-liquid phase change in binary materials, see Prakash [219,220]. In the mid-1980s CHAM also began work on developing a PHOENICS-based CFD model of the HIsmelt process, which involves the direct smelting of iron ore by injecting the iron and coal fines directly into a molten bath, plus the subsequent release and burning of the smelting gas in the top space. Staff movement from CHAM in the early 1990s facilitated the continued refinement of the model by Rio Tinto (Australia), Davis et al. [221]. PHOENICS-based CFD models for materials processing were developed for many other companies, including Arbed Recherche (Luxembourg), Centro Sviluppo Materiali (Italy) and Hoogevens (The Netherlands). During the 1980s and early 1990s, PHOENICS was also used extensively at Massachusetts Institute of Technology by Szekely and co-workers for the development of CFD models of materials-processing operations, A large number of papers were published during this period, for example: Ilegbusi and Szekely [222,223] (tundishes and continuous casting), Cartwright et al. [223] (Czochralski systems) Choo and Szkeley [224] (arc welding). and Saluja et al. [225] (stirred melts). PHOENICS has also been in use at Metallurgical Research Institute AB (Sweden) and the Center for Advanced Study and Research of the National Polytechnic Institute (Mexico) for many years to this day, to conduct research into metals processing, see, for example, Solhed and Jonsson [226] and Rodriguez et al. [227].

Cartesian cut-cell methods for representing complex geometries were in use at CHAM for specific applications during the early 1980s, but it was not until a decade later that Spalding began to initiate a program of work to equip PHOENICS with a generally applicable facility called PARSOL (partial solids). The motivation was to treat imported CAD geometries implicitly and simplify considerably the grid generation associated with using body-fitted non-orthogonal meshes. PARSOL has never been formally published, although some discussion was given in Spalding [228]. The method employs a background Cartesian grid for the majority of the flow domain with special treatments being applied at cells which are cut by solid bodies, thus retaining a boundary-conforming grid. PARSOL is also partially unstructured in that it allows local grid refinement by means of embedded fine-grid regions. The method computes the fractional areas and volumes, and employs a collection of special algorithms for computing interfacial areas, evaluating wall stresses, and for computing advection and diffusion near solid boundaries, etc. Cartesian cut-cell methods have now become a recognized alternative to both structured and unstructured body-conforming meshes, and they are now used in at least three other commercial CFD codes.

During 1993 CHAM implemented into PHOENICS a number of low-Reynolds-number turbulence models that employed normal-wall-distance-based damping functions. It was quickly recognized that the use of conventional search-based geometrical procedures for determining the wall-distance distribution would be far too computationally expensive for handling the arbitrary complex geometries used in industrial applications of PHOENICS. It was then that Spalding proposed the ingenious and extremely economical approach of computing approximate values of the wall distance by solving a Poisson-type transport equation for a scalar variable. Spalding's proposal was mainly intuitive, being based on an analogy with thermal radiation between two plates. This differential-equation based wall-distance algorithm was immediately put to use in PHOENICS for all relevant turbulence closures. The method was only ever formally presented in a poster session at the 10th International Heat Transference Conference, Brighton, by Spalding himself, but thereafter it was exploited, refined and published by Tucker [229,230] and others, and eventually the method or some variant of it found its way into most commercial CFD codes.

The invention of the wall-distance method emerged simultaneously with Spalding's proposal for a zero-equation low-Reynolds-number turbulence model, LVEL, to determine the turbulent kinematic viscosity for situations in which fluid flows through spaces cluttered with many solid objects [231]. In such cases, the grid density between nearby solids is often too coarse for any more advanced turbulence model, such as the two-equation $k$–$\varepsilon$ model, to be meaningfully employed. The turbulent kinematic viscosity was calculated via Spalding's law of the wall [232], which covers the entire laminar and turbulent regimes of the flow. A key element of this model is the Poisson-based differential equation for wall distance mentioned earlier. The LVEL model was implemented in PHOENICS, and used to great practical advantage in electronics-cooling applications, so much so that almost inevitably the model began to appear in other commercial CFD codes, and especially ones dedicated to the thermal design of electronic components and systems. Spalding wrote in his one of his papers [231]

> "*The LVEL model is to be regarded as providing a practical solution to heat-transfer-engineers' problems, and not as one providing new scientific insight.*"

Certainly, the practical usefulness of the model has been demonstrated by many workers, including Rodgers et al. [233], Dhinsa et al. [234], and Choi et al. [235]. The latter report that the LVEL model was as effective as the more advanced two-equation models for simulating rack-mounted servers, with the big advantage being that "significant computation time can be saved (factor of three or higher), especially when conducting transient CFD simulations or when making steady-state runs with different rack settings".

Spalding's ability to recognize the need for engineers in industry to get an adequate solution within reasonable computing time led to the development of the IMMERSOL radiation model. This model was proposed by Spalding in 1994, mainly for economically representing radiation in congested spaces, as found in electronics-cooling applications, and in any other problems where many conducting solids are distributed within the fluid. IMMERSOL, which stands for IMMERsed SOLids, was implemented into PHOENICS by CHAM as an economic option for representing radiation in complex geometries for both optically thick and thin media. The model remains unpublished by Spalding in the open literature, but a description has been given by Rasmussen [236] and Yang et al. [237]. The model involves the solution of a diffusion equation for the radiosity, in which the diffusivity is proportional to the absorption and scattering coefficients of the medium, and the distance between solid walls. The inter-wall distances are computed automatically from a Poisson equation, as explained earlier in connection with computation of wall distances for turbulence modelling. The radiosity equation was devised by simplifying the six-flux model of Hamakar and Schuster, see Spalding [238], by ignoring the directional effects of radiation, but the extension to transparent media was based on physical intuition. IMMERSOL provides an economically realisable approximation to the radiative transfer

equation that gives the exact solution for thermal radiation between two infinitely long parallel plates; and in more complex situations, its predictions are always plausible, and of the right order of magnitude. Successful applications of the model for combustion applications have been reported by both Yang et al. [237,239] and Rasmussen [236], and also by Hien and Istiadji [240] for building ventilation studies with solar radiation. Thus far, IMMERSOL appears to have made little impact on industrial CFD, other than on those organizations who use PHOENICS. One exception is found in the work of Rasmussen [236], who implemented IMMERSOL into another commercial CFD code, STAR-CD, via user programming, and then extended the model to handle wavelength dependence.

PHOENICS stood in the vanguard of practical engineering CFD; for many years it set the standard which the competition attempted to replicate. Inevitably it was imitated, and eventually another CFD code overtook it in terms of sales-volume. Today the CFD practitioner can choose from a number of code-suites, many of which were written by former students of Spalding at Imperial College, or by entrepreneurs who began their initial careers at CHAM and left to form new companies. However PHOENICS also still enjoys widespread use world-wide, and especially so in research circles. It is still the only general-purpose code for which the 'P' (Parabolic) and the 'H' (Hyperbolic) options are appropriate. Indeed the parabolic procedure in PHOENICS was extended by Malin and Spalding [241] to handle under-expanded free jets discharging into subsonic and supersonic free streams, under contract to S&C Thermofluids UK, for use in rocket-exhaust-plume software. This produced solutions much more economically than the elliptic solution procedure. Probably no other commercial code to date has the extensive programmability available to the user. PHOENICS thus is Spalding's own personal, continuously-evolving, living monograph to CFD.

At the 1995 PHOENICS CFD User Conference in Tokyo, Spalding made the following light-hearted observation in terms of CFD T-shirt slogans, on the transition of CFD technology from its research origins in Imperial College to a tool for industrial analysis and design:

| Decade | Slogan | What was happening |
|---|---|---|
| 1960s | We think we can | Imperial College research |
| 1970s | We can! | First applications |
| 1980s | You can too | Start of code-vending industry |
| 1990s | Everyone can | Commercial over-sell |
| 2000s | Everyone will | Web-based services |

Spalding's pioneering role in industrial CFD was summarized by F.C. Lockwood, an original member of the Imperial College team, as follows [242]:

> "*Spalding was able to combine mathematical flair with a copious amount of physical intuition which led to a scientific methodology which was universally appreciated by the engineer at the "sharp end" of real industry problems,*"
>
> and
>
> "*Commercial CFD software developers are not always noted for their generosity of acknowledgement so there is merit in remarking that virtually all of the commercial codes being marketed today owe much to the pioneering work of Spalding and co-workers.*"

## 15. Conclusion

The preparation of this article has been a labour of love on the part of the authors. It is intended as a small tribute to the very large contribution Brian Spalding has made to progress in the fields of mechanical and chemical engineering. Spalding's physical insights, mathematical ability and extraordinary work ethic enabled him to make so many advances in the creation and development of mathematical models to describe turbulence, heat transfer, mass transfer and combustion. His work is characterized by a superb creativity and an extraordinary vision. His ideas often produced a quantum leap in our understanding and predictive capability, and opened the door to new scientific opportunities. He had the desire and ability to generalize a given concept, formula, or procedure. This is what led to far-reaching consequences from his research contributions. The extraordinary depth of knowledge is matched by the enormous breadth of the applications of his work. In addition to his technical work, he was able to communicate his ideas to others effectively through his clear and lucid lectures and writings. His communications skills, combined with being fluent in German and Russian among other languages, enabled him to have a very large impact around the world. His leadership, vision, passion and single-minded obsession also provided industry with multi-purpose tools for the practice of CFD and the development of a suite of tools and services for commercial application. These contributions have had a profound impact in the world of engineering software. He was always a strong advocate for international cooperation and exchange, and had a major influence on the lives and careers of so many of his students and colleagues, among whom we are fortunate to count ourselves. We have tried here to acknowledge some of the achievements of this remarkable man and his remarkable life. Doubtless there will be more in the future.

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