1

Introduction

The study of solutions to systems of semi-linear parabolic partial differential equations has attracted considerable attention over the past fifty years. In the case when the nonlinearity satisfies a local Lipschitz condition, the fundamental theory is well developed (see, for example, the texts of Friedman [21], Fife [20], Rothe [65], Smoller [70], Samarskii *et al.* [67], Volpert *et al.* [72], Leach and Needham [36], and references therein). The situation when the nonlinearity does not necessarily satisfy a local Lipschitz condition is less well studied, but contributions have been made in the case of specific non-Lipschitz nonlinearities which have aided in particular applications (see, for example, Aguirre and Escobedo [5]; Needham *et al.* [36], [54], [29], [33], [40], [41], [42], [43] and references therein), and for the corresponding steady state elliptic problems (see, for example, Stakgold [71], Bandle *et al* [9], [10], [11], [12], [13], Abdullaev [2], [3], [4], [1] and references therein). The aim of this monograph is to exhibit general results concerning semi-linear parabolic partial differential equations that do not necessarily satisfy a local Lipschitz condition. The approach is classical, in the sense that the results relate entirely to the well-posedness criteria for classical solutions, in the sense of Hadamard [39], and the main results are principally established within the framework of real analysis. The approach used to develop the existence theory in this monograph has similarities with the method of successive approximations for systems of first order ordinary differential equations, as detailed in [17] and [16]. Alternative approaches may be possible through the concepts of weak solutions and the framework of semigroup theory. These alternative approaches are amenable, and very effective, in the case of Lipschitz continuous nonlinearities, as exemplified in the monographs by Henry [26] and Pazy [62]. However, the extensions to non-Lipschitz nonlinearities have not been developed and our approach provides an effective development of the classical theory for Lipschitz continuous nonlinearities.

The theory developed in this monograph is applicable to models that arise naturally in many areas of scientific interest. For example, physical, biophysical and environmental modelling gives rise to semi-linear parabolic partial differential equations (often referred to as reaction-diffusion equations) in such areas as population dynamics (see, for example, Levin [37]), the spread of infectious disease (see, for example, Kermack and McKendrick [30], [31] and [32]), smouldering combustion (see, for example, Aris [7] and [8]), isothermal autocatalytic reaction dynamics (see, for example, Gray and Scott [23]), biochemical morphogenesis (see, for example, Murray [52]) and diffusion in complex polymeric materials (see, for example, Edwards [19]). For the purpose of this monograph, we give an introduction based on modelling arising from a chemical kinetics context. Specifically this is motivated by the study of the dynamics of several particular models of autocatalytic chemical reactions under molecular diffusion. These studies can be found in Needham *et al.* [33], [47], [46], [44], [22], [45], [57] and [54]. The aim of this monograph is to develop a generic theory that both encompasses and considerably extends the more specific approaches developed independently in [5], [33] and [54].

The mathematical model concerns the dynamics of an isothermal, autocatalytic chemical reaction scheme with termination, taking place in an unstirred environment and undergoing molecular diffusion. Formally the autocatalytic reaction model is represented by two steps

$$\begin{aligned} A &\longrightarrow B \text{ at rate } k_1 a^q b^p && \text{(autocatalysis)} \\ B &\longrightarrow C \text{ at rate } k_2 b^r && \text{(decay)} \end{aligned}$$

where $p, q, r \in (0, \infty)$ and $k_1, k_2 \in (0, \infty)$ represent the order of each reaction term and the reaction rate constants respectively, whilst a and b represent the concentrations of the reactant A and the autocatalyst B respectively. The chemical C is a stable product of the reaction. At time $\bar{t} = 0$, the autocatalyst is introduced into an expanse of the reactant, which is at uniform concentration $a_0 \geq 0$. This leads to the coupled reaction-diffusion initial boundary value problem, namely,

$$\left.\begin{aligned} \frac{\partial a}{\partial \bar{t}} &= D_a \frac{\partial^2 a}{\partial \bar{x}^2} - k_1 [a^q]^+ [b^p]^+ \\ \frac{\partial b}{\partial \bar{t}} &= D_b \frac{\partial^2 b}{\partial \bar{x}^2} + k_1 [a^q]^+ [b^p]^+ - k_2 [b^r]^+ \end{aligned}\right\} \text{ for } -\infty < \bar{x} < \infty,\ \bar{t} > 0, \tag{1.1}$$

$$a(\bar{x}, 0) = a_0, \quad b(\bar{x}, 0) = b_0 u_0(\bar{x}) \quad \text{for } -\infty < \bar{x} < \infty, \tag{1.2}$$

$$a(\bar{x},\bar{t}) \text{ and } b(\bar{x},\bar{t}) \text{ are bounded as } |\bar{x}| \to \infty \text{ uniformly for } 0 \le \bar{t} \le T \text{ and any } T \ge 0. \tag{1.3}$$

Here $u_0 : \mathbb{R} \to \mathbb{R}$ is bounded and continuous, with bounded derivative and bounded piecewise continuous second derivative, and

$$\sup_{\bar{x}\in\mathbb{R}} u_0(\bar{x}) = 1, \quad \inf_{\bar{x}\in\mathbb{R}} u_0(\bar{x}) = 0. \tag{1.4}$$

The function $u_0 : \mathbb{R} \to \mathbb{R}$ represents the initial concentration distribution of the autocatalyst, with the constant $b_0 \ge 0$ measuring the maximum initial concentration of the autocatalyst, whilst $\bar{x}$ and $\bar{t}$ represent the spatial distance and time. The positive constants D_a and D_b represent the diffusion coefficients for species A and B respectively. Here we define the function $[\ ]^+ : \mathbb{R}^2 \to \mathbb{R}$ for any $a, q \in \mathbb{R}$ to be

$$[\ ]^+(a,q) \equiv [a^q]^+ = \begin{cases} a^q & \text{for } a > 0, \\ 0 & \text{for } a \le 0. \end{cases}$$

When no autocatalysis occurs in (1.1)–(1.3), or equivalently, $k_1 = 0$, then, equation (1.1) and condition (1.2), reduce to

$$a(\bar{x},\bar{t}) = a_0, \quad \frac{\partial b}{\partial \bar{t}} = D_b \frac{\partial^2 b}{\partial \bar{x}^2} - k_2[b^r]^+ \quad \text{for } -\infty < \bar{x} < \infty,\ \bar{t} > 0. \tag{1.5}$$

It is convenient to introduce the function $u : \mathbb{R} \times [0,\infty) \to \mathbb{R}$ and dimensionless variables $\tilde{x}$ and $\tilde{t}$, via

$$b(\bar{x},\bar{t}) = b_0 u(\tilde{x},\tilde{t}), \quad \tilde{t} = \left(\frac{k_2}{b_0^{(1-r)}}\right)\bar{t}, \quad \tilde{x} = \left(\frac{k_2}{D_b b_0^{(1-r)}}\right)^{1/2}\bar{x}. \tag{1.6}$$

On substituting from (1.6) into (1.5), the system (1.1)–(1.3) becomes

$$\frac{\partial u}{\partial \tilde{t}} = \frac{\partial^2 u}{\partial \tilde{x}^2} - [u^r]^+ \quad \text{for } -\infty < \tilde{x} < \infty,\ \tilde{t} > 0, \tag{1.7}$$

$$u(\tilde{x},0) = u_0(\tilde{x}) \quad \text{for } -\infty < \tilde{x} < \infty, \tag{1.8}$$

$$u(\tilde{x},\tilde{t}) \text{ is uniformly bounded as } |\tilde{x}| \to \infty \text{ for each } t \in [0,T] \text{ and any } T > 0. \tag{1.9}$$

The study of the initial-boundary value problem given by (1.7)–(1.9) gives information about the dynamics of the original chemical system in the absence of autocatalysis, which directly motivates the theory of Chapters 6–8 and Chapter 9, Section 9.1. This particular problem has been studied extensively when $r \in [1,\infty)$. However, the case $r \in (0,1)$ has received much less attention.

Returning to the full system (1.1)–(1.3), when the molecular sizes of A and B are comparable, then we can make the simplification

$$D_a = D_b = D. \tag{1.10}$$

We now introduce the functions $\alpha, \beta : \mathbb{R} \times [0, \infty) \to \mathbb{R}$ and dimensionless variables

$$\begin{aligned} a(\bar{x}, \bar{t}) = a_0 \alpha(x, t), \quad b(\bar{x}, \bar{t}) = a_0 \beta(x, t), \\ \bar{x} = \left(\frac{D}{a_0^{p+q-1} k_1} \right)^{1/2} x, \quad \bar{t} = \frac{1}{a_0^{p+q-1} k_1} t. \end{aligned} \tag{1.11}$$

On using (1.10) and (1.11), the initial-boundary value problem (1.1)–(1.3) becomes, in dimensionless form

$$\left.\begin{aligned} \frac{\partial \alpha}{\partial t} &= \frac{\partial^2 \alpha}{\partial x^2} - [\alpha^q]^+ [\beta^p]^+ \\ \frac{\partial \beta}{\partial t} &= \frac{\partial^2 \beta}{\partial x^2} + [\alpha^q]^+ [\beta^p]^+ - k[\beta^r]^+ \end{aligned}\right\} \text{ for } -\infty < x < \infty, \ t > 0, \tag{1.12}$$

$$\alpha(x, 0) = 1, \ \beta(x, 0) = \beta_0 u_0(x) \quad \text{for } -\infty < x < \infty, \tag{1.13}$$

$$\alpha(x, t) \text{ and } \beta(x, t) \text{ are bounded as } |x| \to \infty \text{ uniformly for } t \in [0, T] \text{ and any } T > 0. \tag{1.14}$$

Here we have introduced the dimensionless parameters $\beta_0 = \frac{b_0}{a_0}$ and $k = \frac{k_2}{k_1} a_0^{r-p-q}$. Next, we consider the situation in the absence of the termination step, corresponding to $k = 0$ in (1.12). Additionally, when β_0 is small, we can make the approximation

$$\alpha(x, t) + \beta(x, t) = 1 \quad \text{for } -\infty < x < \infty, \ t \geq 0. \tag{1.15}$$

On substituting from (1.15) into the system (1.12)–(1.14), with $k = 0$, and setting $v = \beta$, leads to the reduced scalar problem

$$\frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial x^2} + [(1 - v)^q]^+ [v^p]^+ \quad \text{for } -\infty < x < \infty, \ t > 0, \tag{1.16}$$

$$v(x, 0) = v_0 u_0(x) \quad \text{for } -\infty < x < \infty, \tag{1.17}$$

$$v(x, t) \text{ is uniformly bounded as } |x| \to \infty \text{ for } t \in [0, T] \text{ and any } T > 0, \tag{1.18}$$

where $v_0 = \beta_0$. The study of problem (1.16)–(1.18) gives information about the dynamics of the original chemical system in the absence of termination

and motivates the theory of Chapter 6, Chapter 8 and Chapter 9, Section 9.3. Furthermore, when we replace the term $(1 - v)^q$ by 1, we obtain the problem which is an approximation to (1.16)–(1.18) when v_0 is small, and this motivates the theory in Chapter 9, Section 9.2.

In this monograph, Chapters 2–5 contain essential introductory material, with new specific extensions which are crucial to later chapters. Chapter 2 is a detailed problem statement concerning the class of problems which this monograph examines, as well as a means of introducing the notation and concepts used throughout. Results are also included to highlight the relationship between certain aspects of interest. Chapter 3 contains maximum principles and contains an extension to the classical parabolic maximum principle, as well as some counterexamples to potentially more general results. Moreover, a result is included to illustrate a violation of the strong maximum principle found in [64] and a suitable amendment is included. Chapter 4 is a summary of well established results regarding the theory for solving *diffusion problems* on $\mathbb{R}$ with bounded initial data. Estimates are also provided which are used in the asymptotic results in Chapter 9, Section 9.2. Chapter 5 introduces the integral equations that arise in the study of *reaction-diffusion problems* in later chapters, together with a class of new "Schauder" type derivative estimates.

Chapters 6–8 provide the general results of the monograph. Chapter 6 is largely a review of the question of well-posedness for the reaction-diffusion problem where the reaction function is *Lipschitz continuous*. Chapters 7 and 8 concern the reaction-diffusion problem when the reaction function is *upper Lipschitz continuous* and *Hölder continuous* respectively. In both of these chapters, conditional well-posedness results are established.

Chapter 9 is dedicated to the study of the three specific problems. The study of the well-posedness and qualitative behavior of solutions to these problems are dealt with for the most part by the theory developed in Chapters 6–8. However the problems in Chapter 9 cannot be fully dealt with by the general theory and problem specific results have also been established.

Chapter 10 discusses possible extensions to the theory developed in the monograph and poses open questions which have arisen through the studies in the monograph.

Throughout the monograph, previously established results that have been proved in the context of the monograph by the authors are marked with (†). When this has not been deemed necessary, instruction or reference to a proof is supplied. All new results are marked with (‡).

2

The Bounded Reaction-Diffusion Cauchy Problem

We begin by introducing the regions in which the forthcoming initial value problems will be defined. Here $T > 0$, $\delta \in [0, T)$ and $X > 0$ and the following sets are introduced:

$$D_T = (-\infty, \infty) \times (0, T],$$

$$\bar{D}_T = (-\infty, \infty) \times [0, T],$$

$$\partial D = (-\infty, \infty) \times \{0\},$$

$$\bar{D}_T^{\delta} = (-\infty, \infty) \times [\delta, T],$$

$$D_T^{\delta, X} = (-X, X) \times (\delta, T],$$

$$\bar{D}_T^{\delta, X} = [-X, X] \times [\delta, T],$$

$$\partial D^{\delta, X} = [-X, X] \times \{\delta\}.$$

The content of the monograph concerns the study of classical solutions $u : \bar{D}_T \to \mathbb{R}$ to the following semi-linear parabolic Cauchy problem;

$$u_t = u_{xx} + f(u); \quad \forall (x, t) \in D_T, \tag{2.1}$$

$$u(x, 0) = u_0(x); \quad \forall x \in \mathbb{R}, \tag{2.2}$$

$$u(x, t) \text{ is uniformly bounded as } |x| \to \infty \text{ for } t \in [0, T]. \tag{2.3}$$

Here, the reaction function $f : \mathbb{R} \to \mathbb{R}$ is prescribed, and the initial data $u_0 : \mathbb{R} \to \mathbb{R}$ is contained in one of the following classes of functions. Firstly, the set of functions $u_0 : \mathbb{R} \to \mathbb{R}$ which are bounded, continuous, with bounded and continuous derivative, and bounded and piecewise continuous second derivative, which is denoted as

$$\text{BPC}^2(\mathbb{R}).$$

Secondly and thirdly, the two subsets of $\mathrm{BPC}^2(\mathbb{R})$, the first of which contains only non-negative functions $u_0 \in \mathrm{BPC}^2(\mathbb{R})$, and the second, which contains only non-negative functions $u_0 \in \mathrm{BPC}^2(\mathbb{R})$ but excludes the zero function, which are denoted, respectively, by

$$\mathrm{BPC}^2_+(\mathbb{R}) \text{ and } \mathrm{BPC}^2_{+'}(\mathbb{R}).$$

The partial differential equation (PDE) (2.1) is generally referred to as a *reaction-diffusion equation*, and the initial value problem given by (2.1)–(2.3) will be referred to throughout the monograph as the *bounded, reaction-diffusion Cauchy problem*, abbreviated to (B-R-D-C). Moreover, throughout the monograph, we adopt the following classical definition of solution to (B-R-D-C):

Definition 2.1 A solution to (B-R-D-C) is a function $u : \bar{D}_T \to \mathbb{R}$ which is continuous and bounded on $\bar{D}_T$ and for which u_t, u_x and u_{xx} exist and are continuous on D_T. Moreover $u : \bar{D}_T \to \mathbb{R}$ must satisfy each of (2.1)–(2.3). ⌟

The questions addressed in this monograph concern the global well-posedness of (B-R-D-C) in the sense of Hadamard [39]. In particular, for a given $f : \mathbb{R} \to \mathbb{R}$, we seek to establish,

(P1) (Existence.) for each $u_0 \in \mathcal{A} \subset \mathrm{BPC}^2(\mathbb{R})$, there exists a solution $u : \bar{D}_T \to \mathbb{R}$ to (B-R-D-C) on $\bar{D}_T$ for each $T > 0$,

(P2) (Uniqueness.) whenever $u : \bar{D}_T \to \mathbb{R}$ and $v : \bar{D}_T \to \mathbb{R}$ are solutions to (B-R-D-C) on $\bar{D}_T$ for the same $u_0 \in \mathcal{A} \subset \mathrm{BPC}^2(\mathbb{R})$, then $u = v$ on $\bar{D}_T$ for each $T > 0$,

(P3) (Continuous Dependence.) given that (P1) and (P2) are satisfied for (B-R-D-C), then given any $u_0' \in \mathcal{A} \subset \mathrm{BPC}^2(\mathbb{R})$ and $\epsilon > 0$, there exists a $\delta > 0$ (which may depend on u_0', T and ϵ) such that for all $u_0 \in \mathcal{A} \subset \mathrm{BPC}^2(\mathbb{R})$, then

$$\sup_{x\in\mathbb{R}} \left|u_0(x) - u_0'(x)\right| < \delta \implies \sup_{(x,t)\in\bar{D}_T} \left|u'(x,t) - u(x,t)\right| < \epsilon$$

where $u : \bar{D}_T \to \mathbb{R}$ and $u' : \bar{D}_T \to \mathbb{R}$ are the solutions to (B-R-D-C) corresponding respectively to $u_0, u_0' \in \mathcal{A} \subset \mathrm{BPC}^2(\mathbb{R})$. This must hold for each $T > 0$.

When the above three properties (P1)–(P3) are satisfied by (B-R-D-C), then (B-R-D-C) is said to be *globally well-posed* on $\mathcal{A}$. Moreover, when (P1)–(P3) are satisfied by (B-R-D-C) and the constant δ in (P3) depends only on u_0' and ϵ (that is, being independent of T), then (B-R-D-C) is said to be *uniformly*

globally well-posed on $\mathcal{A}$. When one or more of the properties (P1)–(P3) are not satisfied, then (B-R-D-C) is said to be *ill-posed* on $\mathcal{A}$. In addition to well-posedness, we shall address some fundamental qualitative features of solutions to (B-R-D-C).

In conjunction with solutions, we introduce two concepts which will be used throughout the monograph.

Definition 2.2 Let $\overline{u}$, $\underline{u} : \bar{D}_T \to \mathbb{R}$ be continuous on $\bar{D}_T$ and such that $\underline{u}_t$, $\underline{u}_x$, $\underline{u}_{xx}$, $\overline{u}_t$, $\overline{u}_x$, and $\overline{u}_{xx}$ exist and are continuous on D_T. Suppose further that

$$N[\,\overline{u}\,] \equiv \overline{u}_t - \overline{u}_{xx} - f(\overline{u}) \geq 0 \ \text{ on } D_T,$$

$$N[\,\underline{u}\,] \equiv \underline{u}_t - \underline{u}_{xx} - f(\underline{u}) \leq 0 \ \text{ on } D_T,$$

$$\underline{u}(x,0) \leq u_0(x) \leq \overline{u}(x,0); \ \ \forall\, x \in \mathbb{R},$$

$$\underline{u} \text{ and } \overline{u} \text{ are uniformly bounded as } |x| \to \infty \text{ for t } \in [0,T].$$

Then on $\bar{D}_T$, $\underline{u}$ is called a *regular sub-solution* (R-S-B) and $\overline{u}$ is called a *regular super-solution* (R-S-P) to (B-R-D-C). ⌟

In addition, we require the concept of (B-R-D-C) being *a priori bounded*. This is formalised in the following definition.

Definition 2.3 Suppose that, for (B-R-D-C), we can exhibit a constant $l_T > 0$ for each $0 \leq T \leq T^*$ (and some $T^* > 0$) which depends only upon T and $\sup_{x\in\mathbb{R}} |u_0(x)|$, and which is non-decreasing in $0 \leq T \leq T^*$. Suppose, furthermore, that if $u : \bar{D}_T \to \mathbb{R}$ is any solution to (B-R-D-C) on $\bar{D}_T$, then it can be demonstrated that

$$\sup_{(x,t)\in\bar{D}_T} |u(x,t)| \leq l_T,$$

for each $0 \leq T \leq T^*$. We say that (B-R-D-C) is *a priori bounded* on $\bar{D}_T$ for each $0 \leq T \leq T^*$, with bound l_T. ⌟

In (B-R-D-C), the function $f : \mathbb{R} \to \mathbb{R}$ is referred to as the reaction function, and throughout the monograph we will restrict attention to those reaction functions f from one or more of the following classes of functions. The first class of functions is defined as,

Definition 2.4 A function $f : \mathbb{R} \to \mathbb{R}$ is said to be *Lipschitz continuous* if for any closed bounded interval $E \subset \mathbb{R}$ there exists a constant $k_E > 0$ such that for all $x, y \in E$,

$$|f(x) - f(y)| \leq k_E |x - y|.$$

The set of all functions $f : \mathbb{R} \to \mathbb{R}$ which satisfy this definition will be denoted by L. ⌟

For example, any differentiable function $f : \mathbb{R} \to \mathbb{R}$ which has bounded derivative on every closed bounded interval $E \subset \mathbb{R}$ is such that $f \in L$. It is also clear that every function $f \in L$ is continuous. This class of functions has been mentioned first, due to the classical theory of bounded reaction-diffusion Cauchy problems being largely restricted to the case of $f \in L$. The second class of functions which we introduce is parameterised by a real number $\alpha \in (0, 1]$ and is defined as,

Definition 2.5 A function $f : \mathbb{R} \to \mathbb{R}$ is said to be *Hölder continuous of degree* $\alpha \in (0, 1]$ if for any closed bounded interval $E \subset \mathbb{R}$ there exists a constant $k_E > 0$ such that for all $x, y \in E$,

$$|f(x) - f(y)| \leq k_E |x - y|^\alpha.$$

The set of all functions $f : \mathbb{R} \to \mathbb{R}$ which satisfy this definition will be denoted by H_α (note that $H_1 = L$). ⌟

Any differentiable function $f : \mathbb{R} \to \mathbb{R}$ which has bounded derivative on every closed bounded interval $E \subset \mathbb{R}$ is contained in H_α (for every $\alpha \in (0, 1)$) and every function in H_α is continuous (for any $\alpha \in (0, 1)$). The third class of functions which will be considered in the monograph is defined as,

Definition 2.6 A function $f : \mathbb{R} \to \mathbb{R}$ is said to be *upper Lipschitz continuous* if f is continuous, and for any closed bounded interval $E \subset \mathbb{R}$, there exists a constant $k_E > 0$ such that for all $x, y \in E$, with $y \geq x$,

$$f(y) - f(x) \leq k_E (y - x).$$

The set of all functions $f : \mathbb{R} \to \mathbb{R}$ which satisfy this definition will be denoted by L_u. ⌟

Also, for any closed bounded interval $E \subset \mathbb{R}$, any $f \in L_u$ is bounded, and, in particular, setting $E = [a, b]$, we have

$$f(b) + k_E(x - b) \leq f(x) \leq f(a) + k_E(x - a); \ \forall x \in [a, b]. \tag{2.4}$$