ANALYSIS OF REACTION-DIFFUSION SYSTEMS FOR FLAME CAPTURING IN TYPE Ia SUPERNOVA SIMULATIONS

A DISSERTATION SUBMITTED TO
THE FACULTY OF THE DIVISION OF THE PHYSICAL SCIENCES
IN CANDIDACY FOR THE DEGREE OF
DOCTOR OF PHILOSOPHY

DEPARTMENT OF PHYSICS

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CHICAGO, ILLINOIS
JUNE 2009
ABSTRACT

We present a study of numerical behavior of a thickened flame used in Flame Capturing (FC, Khokhlov (1995)) for tracking thin physical flames in deflagration simulations. This technique, used extensively in astrophysics, utilizes artificial flame variable to evolve flame region, width of which is resolved in simulations, with physically motivated propagation speed. We develop a steady-state procedure for calibrating flame model used in FC, and test it against analytical results. Original flame model is properly calibrated with taking matter expansion into consideration and keeping artificial flame width at predetermined value regardless of expansion.

We observe numerical noises generated by original realization of the technique. Alternative artificial burning rates are discussed, which produce acceptably quiet flames (relative dispersion in propagation speed within 0.1\% at physically interesting ratios of fuel and ash densities).

Two new quiet models are calibrated to yield required “flame” speed and width, and further studied in 2D and 3D setting. Landau-Darrieus type instabilities of the flames are observed. One model also shows significantly anisotropic propagation speed on the grid, both effects increasingly pronounced at larger matter expansion as a result of burning; these 2D/3D effects make that model unacceptable for use in type Ia supernova simulations at fuel densities below about 100 tons per cubic centimeter. Another model, first presented here, looks promising for use in flame capturing at fuel to ash density ratio of order 3 and below, the interval of most interest for astrophysical applications. No model was found to significantly inhibit LD instability development at larger expansions without increasing flame width. The model we propose, “Model B”, yields flames completely localized within a region 6 cells wide at any expansion.

We study Markstein effect (speed of the flame dependence on its curvature) for flame models described, through direct numerical simulations and through quasi-steady technique developed. By comparing results obtained by the 2 approaches we demonstrate that Markstein effect dominates instability effects on curved flame speed for Model B in 2D simulations for fuel to ash density ratio of about 2.5 and below. We find critical wavelength of LD instability by direct simulations of perturbed nearly planar flames; these agree with analytical predictions with Markstein number values found in this work. We conclude that the behavior of model B is well understood, and optimal for FC applications among all flame models proposed to date.
ACKNOWLEDGMENTS

I am grateful to Alexei Khokhlov for proposing original problem of correct calibration of his flame model, which over time evolved into extensive study of various aspects of behavior of flames. His encouraging comments, stimulating discussions on various astrophysical issues, references suggested — especially at the beginning of the project — are greatly appreciated. Most numerical simulations presented here were performed with code ALLA, in creating which Alexei was a main contributor.

Thanks to the Committee members: Juan Collar, Robert Rosner and Thomas Witten, whose comments contributed to shaping the final form of the thesis.

Thanks to FLASH Center for numerous talks and meetings organized over the years, which broadened my horizons in astronomy, astrophysics and computational physics; and for supporting my graduate study. Alan Calder, Tridivesh Jena, Dean Townsley helped me with basics of FLASH code operation, which is appreciated.

Thanks to Alexei Poludnenko for numerous inspiring conversations on variety of scientific and general topics, and for great job in maintaining computer cluster.

Numerous seminars, presentations, colloquia at Physics, Math, Astronomy and Astrophysics Departments of the University of Chicago were encouraging and helped to keep motivation.

Thanks to my friends at the University of Chicago and beyond. In particular, I am indebted to Lenya Malyshkin and Sasha Paramonov for their help during my last days in Chicago.

Thanks to my family.
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CHAPTER 1
INTRODUCTION

In the thesis we study features of propagating flame solutions in reaction-diffusion (RD) systems. Such flames are ubiquitously observed in chemical combustion in terrestrial experiments and in industry, as well as in certain astrophysical phenomena, with fast composition transformation taking place in nuclear deflagration fronts propagating through stellar material. For most of the study we concentrate on a few specific RD models used in, or proposed here for use in simulations of deflagration phase in type Ia supernova (SN Ia; plural SNe Ia) phenomenon. An important applied goal of the study is to propose an optimal flame model to be used in the simulations, the one that reliably reproduces expected physical propagation of a deflagration front in SN Ia problem, without introducing unphysical numerical artifacts, such as numerical noises, excessive front instabilities and anisotropic behavior related to computation grid.

We start with a brief overview of SN Ia phenomenon, providing motivation for the study, and discussing general physics of flames in this example system. We then proceed to describing techniques currently used for numerical simulations of SN Ia. The chapter is concluded with the list of problems the current simulations face that we address in this work, and with more detail on organization of the thesis.

1.1 Supernovae: observations

Extreme cases of variable stars, which are now classified as novae and supernovae, attracted human attention since ancient times. The first accurate record of such an event, with documented dates (185 AD) and position (close to $\alpha$ Centauri) is due to Chinese astronomers (Zhao et al. (2006)). Crab Nebula M1 and the famous short-period pulsar within are remnants of another supernova, observed by Chinese, Japanese and Arab astronomers in 1054; for 23 days it was bright enough to be visible in daylight, and at nights it was visible with naked eye for 653 days. In 1572 Tycho Brahe measured parallax of another star of this class (to find no detectable parallax); he also recorded its dimming with time. That was the first well-documented supernova in western world; Brahe’s book, “De Stella Nova”, gave rise to the name we currently use for a different explosive phenomenon, much more frequent and dim than supernovae.

There were more than a hundred classical novae (now understood as a result of explosive burning of accreted hydrogen-helium fuel on a surface of a White Dwarf star in binary systems, when certain critical mass of the fuel is accumulated) studied by 1919, when Lundmark suggested that the distance to M31, “Andromeda Nebula”, was $7 \times 10^5$ light years (at that time most astronomers believed that everything
observed on the sky belonged to our Galaxy). Even with this significantly underestimated distance it followed that S Andromedae explosion of 1885 was extragalactic, and hence was more luminous than classical novae studied by about 3 orders of magnitude (Lundmark (1920)). With improved distance measurements Baade & Zwicky (1934) suggested to differentiate between novae and supernovae, in the way as used nowadays.

Typical supernova brightness rises rapidly for a few weeks, reaches “maximum light”, then drops within months, approximately exponentially after a few weeks of less regular transient dimming. At maximum light SNe are among the brightest objects in the Universe, often shining brighter than the whole host galaxy. Zwicky (1938) proposed collapse of a star made of ordinary matter into a neutron star as a mechanism for SN phenomenon; currently accepted scenario of certain types of core-collapse supernovae is based on that idea. All supernovae are understood now to be a result of cataclysmic event happening to some stars in late stages of their evolution, after almost all hydrogen and helium are transformed into carbon and heavier elements. As observed energy emitted within a few weeks following such an event (around maximum light), is comparable to energy produced by the Sun over its multi-billion year history, it is clear that SN event must involve drastic transformation of the whole star structure. In fact, the transformation of most of the star composition takes just a few seconds based on current understanding of the physics of SNe.

Historically supernovae are categorized into a few types based on their spectral features. Supernovae of type II show hydrogen absorption lines in the spectrum near maximum luminosity, those of type I show no hydrogen. Supernovae of type I showing strong Si II lines belong to class Ia; those with no silicon lines are further subdivided into types Ib and Ic if they show or lack helium lines, respectively.

Observationally SNe Ia are special in that vast majority of them show close peak luminosity and light curve decline features, whereas variety within other types is significant. Typical SN Ia light curve (brightness vs time) shows initial rise interval about 20 days long, followed by about as fast decline, about 3 magnitudes within a few weeks, then dimming more slowly by about a magnitude per month. For most spectroscopically normal SNe Ia the absolute bolometric magnitude at maximum light lie in narrow interval from $-19.4^m$ to $-18.7^m$. Phillips (1993) observed that this scatter in peak luminosities is correlated with light curve width (characterized by $\Delta m_{15}(B)$, star magnitude drop within 15 days after maximum light); this Phillips relation makes it possible to accurately predict SN Ia absolute magnitude based on observed dimming rate. Coupled with extreme brightness of supernovae this makes SN Ia excellent standard candles for probing cosmological distances. Peculiarities in observed SN Ia magnitude as a function of their redshift was a first indication that the Universe is expanded with (positive) acceleration (see Leibundgut (2001) for a review).
SNe Ia also differ from SNe of different types in their environment: Ia is the only supernova type observed in elliptical galaxies, although they still occur about twice more frequently in younger stellar populations in spiral and irregular galaxies (Cappellaro et al. (1997)).

These features, together with low luminosities of SN Ia in radio, X-ray and gamma bands suggest less massive progenitor of SNe Ia than those of other types of supernovae, and no collapse happening in the process of explosion. All other supernova types are believed to involve core collapse to a neutron star or a black hole as a main source of energy powering disruption of and energy deposition into the envelope.

1.2 SNe Ia: physical models

Below we briefly overview physical models of SN Ia, mostly paying attention to physical issues relevant for our study. See, e.g., Hillebrandt & Niemeyer (2000) for more detail on explosion models.

1.2.1 Overview

SNe Ia are believed to be a result of thermonuclear explosion of a White Dwarf (Hoyle & Fowler (1960), Arnett (1969)), a late stage of evolution of light stars, with main sequence mass below about 8 solar masses. All models involve heavy White Dwarfs (WDs), with masses close to or exceeding solar mass $M_\odot$. Such WDs are formed from contracted central parts of stars after hydrogen and helium burning there is complete and H/He-rich shell is dissipated in space. They are composed of $^{12}$C and $^{16}$O mostly, and are supported by the cold pressure of degenerate electrons. WDs with smaller amounts of carbon, but rich in heavier elements, $^{20}$Ne and $^{24}$Mg, are also candidates to undergo a thermonuclear explosion, however some calculations (Gutierrez et al. (1996)) indicate that core collapse is a probable outcome of near-central ignition in such WDs.

For all specific models (briefly discussed below) not overtly contradicting observations successful result of the explosion is stellar material transformed mostly into $^{56}$Ni with considerable amount of intermediate-mass elements (Si, S, Ca) within about 3 s of proper explosion; enough energy is released for total disruption of the WD. Explosion itself is practically invisible due to opacity of dense hot ashes of the explosion; significant part of the released energy is spent to overcome gravitational potential of the compact star, with excess transformed into kinetic energy of expanding material. A few days after explosion, expanding envelope starts looking bright to an external observer, though it remains optically thick until much later times. Double $\beta$-decay of $^{56}$Ni to $^{56}$Co ($t_{1/2} = 6.08$ d) and then to stable $^{56}$Fe ($t_{1/2} = 77.2$ d) powers the light curve (Truran et al. (1967), Colgate & McKee (1969)), that is it heats the expanding gas, which captures emitted in the decay positrons and $\gamma$-quanta and eventually
reemits light outside, mostly in optical band. Both the initial light-curve decline rate (governed by slow diffusion of light out of the gas nebula) and peak luminosity (Arnett (1982)) turn out to be proportional to amount of $^{56}\text{Ni}$ produced, thus providing an explanation for Phillips relation.

Specific models proposed differ in particulars of progenitor, ignition and burning mechanism. The most natural model to account for uniformity of most SN Ia events, single-degenerate scenario with nearly Chandrasekhar mass $M_{\text{Ch}}$ (the maximal mass of the WD that degenerate electron pressure can support, Chandrasekhar (1931); about $1.4M_\odot$), involves ignition near the center of a heavy WD as a result of thermonuclear runaway, readily happening in highly-degenerate fuel (C+O) in central part of a WD with near-critical mass. The progenitor WD is believed to be formed with lower mass, and to have its mass increased by accretion from a companion giant or main-sequence star. Parameters of the close binary system must be rather special so that accreting hydrogen or helium steadily burned into C/O on the surface of a WD, without nova outbursts (which do not on average lead to increase in a WD mass); cf. Nomoto et al. (2000) for study of the accretion process.

The amount of nickel produced, and thus the maximal luminosity (if explosion does unbind the WD) is likely to depend on WD composition, rotation, and on specifics of explosion process, thus leading to variation in nickel mass produced. In the model of Arnett (1969) explosion starts as detonation, and it is in this detonation front sweeping through entire star where all “fuel”, C+O, is transformed into ash; the latter consists almost completely of nickel after detonation at original high density of WD material. This contradicts observations, which show a few tenths of solar mass of intermediate mass elements produced by all SNe Ia. Pure detonation model (in near-Chandrasekhar mass WD) is thus ruled out by observations (Arnett (1974), Ostriker et al. (1974)). It is believed that “explosion” in a single degenerate near-$M_{\text{Ch}}$ model is started as deflagration, possibly turning into detonation at a later stage. We will discuss this in more detail in the next section.

Other class of models involve WDs with masses substantially below $M_{\text{Ch}}$. While such lighter WDs (still massive enough to consist mostly of carbon/oxygen) will not self-ignite, detonation front may be sustained once initiated, according to simulations. Woosley & Weaver (1994), Livne & Arnett (1995) present 1D and 2D simulations, in which detonation is initiated on the surface of C/O subchandrasekhar WD, by self-detonating (through runaway at the bottom) accreted helium shell of $\sim 0.2M_\odot$. Detonations at lower densities in such lighter WDs can produce significant amounts of intermediate-mass elements, though some features observed in simulations (like large amounts of $^{44}\text{Ti}$ produced) are not supported by observations. Models of this type are attractive as binary systems containing lower mass WDs are more abundant; however accumulation of significant mass of He is still required for the mechanism to work; also, due to a range of possible progenitor masses there is no natural explanation for uniformity of SN Ia peak luminosities. Finally, simulations performed in 2D with
postulated axial symmetry are just not reliable, as 3D simulations of the last decade suggest.

In double degenerate scenario (Webbink (1984), Iben & Tutukov (1984)) ignition is initiated by collision of 2 sub-$M_{\text{Ch}}$ WDs. This scenario requires very close binary system of WDs orbiting around each other: their separation must not exceed $\sim 10^6$ km so that the merging happened on cosmological timescales, assuming gravitational radiation as the main damping mechanism. Like the model in the previous paragraph there is no special mass for merging system, thus significant dispersion in maximum luminosities is to be expected. Such non-standard mechanisms may be an explanation for a small number of SNe Ia with peculiar spectra and substantially high or low peak luminosity.

1.2.2 Deflagration and detonation in a White Dwarf: physics

As reviewed in the previous section, nuclear explosion of a near-$M_{\text{Ch}}$ WD is currently considered the best explanation for SN Ia. What is usually loosely referred to as “explosion” physically corresponds to one of 2 possible modes of fast fuel transformation (through a network of thermonuclear reactions) into ash, in thin front propagating through the system (WD). Reaction rates show sharp dependence on temperature, of Arrhenius type. Temperature in the reaction zone (within the front) must be raised to approximately reaction activation energy for the reaction to progress with substantial rate.

Detonation mode is characterized by supersonic front speed; adiabatic compression by significant pressure jump across the front is the mechanism raising the temperature high enough for reactions to proceed. Heat released in the reactions sustains the shock wave propagation. Due to fast detonation front velocity, if detonation is initiated near WD center as the start of the explosion, the whole WD will be swept by the front at nearly original high density — density distribution has just no time to change. Reaction goes all the way through nuclear statistical equilibrium (NSE) composition at densities above $5 \times 10^3\text{g cm}^{-3}$; and this composition is mostly iron-group elements (having the highest binding energies per nucleon) at high fuel densities. This is why too little lighter elements is produced in pure detonation model.

In deflagration mode a flame (thin zone with large gradients of temperature, density, composition; it contains reaction zone) propagates into the fuel by diffusion-reaction mechanism. Temperature is raised in front of the flame due to heat conduction from the hot reaction zone. Temperature distribution has characteristic for diffusion processes exponential tail deep into cold fuel; right in front of the reaction zone (where still the fuel is not depleted in the reaction) the temperature continuously approaches high flame temperature, leading to high reaction rate; flame this way propagates forward. Thermal energy released in reaction zone prevents temper-
ature profile from smearing out by heat conduction; steady solutions (of the form of a kink wave) typically exist describing propagating flame with constant in time distribution of physical quantities within, in the flame rest-frame. See Chapter 2 for details; Fig. 2.1 shows ash fraction distribution in one particular flame model.

Species diffusion, and their production/depletion in the reaction zone contribute to distribution of composition and temperature near the flame (see Sec. 5.1 below for details). In terrestrial combustion in nearly ideal gases burning is affected to approximately the same degree by diffusion as it is by heat conductivity, as Lewis number (ratio of heat diffusivity to matter composition diffusivity) $Le \approx 1$. For WD matter thermal conductivity by far dominates other transfer phenomena, $Le \sim 10^7$, thus species diffusion plays negligible role in flame propagation.

Laminar flame speed as estimated in Timmes & Woosley (1992) depends on fuel composition (that is local WD composition in front of the flame) and density; it is about $80 \text{ km s}^{-1}$ in central region of $0.5\text{C}+0.5\text{O}$ near-M$_{\text{Ch}}$ WD (central density $\rho_{\text{fuel}} \approx 2 \times 10^9 \text{ g cm}^{-3}$) and lower at smaller densities in outer layers. This velocity can be roughly estimated by equating characteristic energy release timescale,

$$t_{\text{reac}} \approx 1/R$$

with heat diffusion timescale (assuming comparable or smaller contribution to flame dynamics from species diffusion, i.e. $Le \approx 1$ or greater)

$$t_{\text{diff}} \approx \frac{W^2}{\kappa}.$$  

$R$ here stands for some characteristic value of reaction rate in flame zone, such that the average energy release rate in the flame $\langle dQ/dt \rangle = R q$, $q$ being total heat release of the reaction; $\kappa = \lambda/(c_V \rho)$ is temperature diffusivity coefficient ($\lambda$ meaning heat conductivity, $\rho$ density and $c_V$ specific heat). This balance of timescales determines flame width $W$, which further provides rough estimate for laminar flame speed:

$$W \approx \sqrt{\kappa/R}, \quad S_l \approx W/t_{\text{reac}} \approx \sqrt{\kappa R}.$$  

See Zeldovich et al. (1985); Williams (1985) for more accurate estimates, and for more on physics of deflagration.

1.2.3 Pure deflagration models

Whether deflagration alone can account for observable features of SNe Ia is not straightforward to answer. Laminar flame speed is far less than sound speed anywhere in the WD, thus flame propagation is nearly isobaric; star structure changes as heat is released in the flame, WD expands, this hydrodynamic evolution must be
computed simultaneously, coupled to flame propagation calculations. Early 1D simulations suggested that fast WD expansion after deflagration sets in quenches burning too early, so that not enough energy is released to unbind the star; WD contracts back after burning stops. It was understood, however, that in reality the flame will never propagate as an ideal spherical flame with its laminar burning speed, due to instabilities discussed below.

It is known that deflagration fronts are subject to a number of instabilities, which can drastically affect flame propagation. As soon as transverse flame dimensions exceed characteristic instability scales $\lambda_{cr}$ flame surface starts developing various features (bubbles, wrinkles — the geometry depends on specific instability involved) increasing its surface compared to a smooth surface stable laminar flame would have had; this effectively increases integral burning rate. In flamelet regime, that is when characteristic spatial scale of flame surface perturbations by flame instabilities and background turbulence significantly exceeds laminar flame width, kinetics of the burning (and hence distribution of physical quantities) within the flame is not affected significantly; integral burning rate is increased approximately in proportion to flame surface increase (compared to stable laminar burning). When a flame is perturbed on scales comparable to or less than its laminar width burning description based on laminar flame physics becomes not applicable, the flame is generally torn apart; such regime is called distributed burning (Damköhler (1940)).

For nuclear deflagration in degenerate WD matter, where kinematic viscosity and species diffusivity are negligible compared to temperature diffusivity $\kappa$, hydrodynamic instability of the type (abbreviated LD below) studied by Landau (1944), Darrieus (1938) is important. Besides, the flame is subject to Rayleigh-Taylor (RT) instability (basically a buoyancy instability — occurring when lower density reaction products support denser cold fuel above in WD gravitational field, directed towards its center), and to Kelvin-Helmholtz (KH) instability, perturbing shear flow interfaces, like on sides of rising RT bubbles. LD instability is most important on scales comparable with flame width. Such scales are never resolved in full star simulations (flame width is submillimeter for most of deflagration phase Timmes & Woosley (1992)). On the largest scales RT instability dominates, driving hydrodynamics on the scale of the star. See Khokhlov (1994, 1995) for features of RT-driven burning in cylinders with uniform gravitational field, and in 3D SN Ia simulations. One result of studies in cylindrical geometry important in applications (see next section) is that after certain transient time steady (in average) burning sets in uniform gravity driven RT burning, with integral burning velocity (“turbulent flame speed”, $S_t$) depending only on geometry of the cylinder cross-section, and independent of laminar flame speed.

$$S_t \approx 0.5 \sqrt{Ag \Delta}$$ (1.1)

is the value confirmed in Khokhlov (1995), Zhang et al. (2007) as reasonably accurate. $\Delta$ here stands for linear scale of cylinder cross-section (in the cited works horizontal
cross-section was a square with side $\Delta$; $A$ denotes Atwood number for fuel–ash,

$$A = \frac{(\rho_{\text{fuel}} - \rho_{\text{ash}})}{(\rho_{\text{fuel}} + \rho_{\text{ash}})}.$$  

(1.2)

$g$ stands for gravitational acceleration.

The smaller the laminar speed the more intricate surface of the flame develops, its area in steady regime scaling inversely proportional to $S_l$, laminar speed of the flame. If $S_l$ is increased, on the other hand, the surface becomes smoother; when $S_l > S_t$ (as given in (1.1)) flame is essentially flat and propagates with its laminar speed; that is for any geometry of the system flames with large enough $S_l$ are stable to RT. See Khokhlov (1995) for more on self-regulation mechanism behind this behavior; qualitatively, for flames with larger laminar speed laminar burning overruns slower developing smaller RT bubbles, thus only larger-scale bubbles (which rise faster) develop — the surface is polished by burning on lower scales.

In non-steady 3D setting in deflagrating WD characteristic large scale burning speed $S_l$ on large scales increases as the flame gets farther from the WD center, as Atwood number, gravity and available tangential dimension increase; in addition, the instability had been allowed more time to develop before the flame got to such larger radius. Laminar flame speed, on the other hand, rapidly decreases, as fuel density decreases. Hence, early 1D simulations grossly underestimated total burning rate, except at the very center of the WD. 1D models are used for certain purposes till now, however the flame speed is prescribed based on estimates of $S_l$ from 3D analysis. Often this burning rate is being left as a (time dependent) free parameter, tuned to get desired features on the output of the simulation, close to observations; some calculations of this type are notably successful in yielding results closely resembling observed SN Ia features (Nomoto et al. (1984)).

Real 3D simulations are needed to judge about viability of a pure deflagration model. These still use artificial techniques to propagate the flame with right velocity (improving one of such techniques, proposed in Khokhlov (1994), is a subject of this thesis) as the scales physically governing flame propagation are not resolved in any WD-scale 3D simulations. However the techniques aim to get the flame propagating with correct, physically motivated effective speed to reproduce, on resolved scales, speed of real thin physical flame; no tuning of flame speed with the purpose of getting particular output results is used. We will discuss the techniques used in the next section; more detail on implementation and the results may be found in Khokhlov (2000), Gamezo et al. (2003), Gamezo et al. (2005), Reinecke et al. (2002a), Niemeyer et al. (2002).

No consensus exists right now whether deflagration alone may explain a normal type Ia supernova. With currently used subgrid models, prescribing flame speed so that to get total burning rate as the physical one (as the latter is currently understood), of submillimeter-thick nuclear flame wrinkled on unresolved scales, different
groups get enough energy to unbind the WD, for near-central single-spot ignition. The amount of energy released in such deflagration models is still lower than in normal SNe Ia, as is amount of iron-group elements produced. Significant amount of unburned carbon and oxygen remains close to the center of the star, a result of sinking RT fingers of cold fuel. After homologous expansion of unbound WD sets in (about 10 seconds after original ignition) these fingers are observed as large amounts of unburned material expanding with low velocities; on the other hand in real SNe Ia light elements are observed almost exclusively in outer layers of expanding nebula, that is having largest expansion speeds.

Attempts were undertaken (Röpke & Hillebrandt (2005)) to fix some of these shortcomings with extending burning simulation at lower densities, in distributed burning regime (starting at densities below about $10^7$ g cm$^{-3}$, when flame preheating zone becomes wider than Gibson scale.\footnote{This is the scale on which average turbulent velocity fluctuations are equal to the laminar flame speed. On lower scales the turbulent fluctuations are smaller, therefore flame propagation is insensitive to turbulence on such lower scales. Above Gibson scale flame surface is bent and stretched by background turbulent flows. The turbulence on all scales is mostly generated (through Kolmogorov cascade) by large-scale RT motions, augmented with vorticity generated by KH instability.}

Another (effective) approach (Travaglio et al. (2004); Röpke et al. (2007)) is based on multipoint ignition. Igniting at several points distributed in the central part of a WD simultaneously reduces the amount of unburnt fuel near the center and increases the amount of nickel produced. Say, simultaneous ignition in 1600 spherical spots in Röpke et al. (2007) resulted in asymptotic kinetic energy of ejecta of $8.1 \times 10^{50}$ erg, with $0.606 \, M_\odot$ of iron group elements produced, including $0.33 \, M_\odot$ of $^{56}$Ni. Corresponding results in Reinecke et al. (2002b) with single spot central ignition (albeit smaller resolution) are $4.5 \times 10^{50}$ erg, $0.5 \, M_\odot$ and $0.3 \, M_\odot$. Simulation in Travaglio et al. (2004), in one octant of a full WD (octahedral symmetry assumed) with 30 bubbles (larger than in Röpke et al. (2007), 10 km radius vs 2.6 km; and located closer to WD center) ignited at $t = 0$ resulted in $6.5 \times 10^{50}$ erg asymptotic kinetic energy of ejecta and $0.418 \, M_\odot$ of $^{56}$Ni produced. Kinetic energy of ejecta of a typical observed SN Ia is slightly above $10^{51}$ erg. Exact pre-explosion conditions (smoldering phase) at the center of a WD are not known well, so it is not obvious if single point ignition is the best choice of initial conditions. Yet significant dependence on this choice of initial conditions is noteworthy, even though dispersion in Ni masses quoted above would lead to dispersion in brightness within $0.8^m$, comparable to dispersion among observed Ia’s.

### 1.2.4 Delayed detonation models

The best fit with observations is obtained in hybrid models, where “explosion” starts as deflagration, and later on detonation is triggered in some spot of the WD pre-
expanded during the deflagration phase. Detonation happening at lower densities under such a scenario produces sufficient amount of intermediate mass elements (in outer layers of preexpanded WD), transforms RT fingers of fuel near WD center into iron-group elements (together with the whole dense central part: detonation front is smooth, on scales characteristic for RT instability, in contrast with intricately corrugated deflagration front surface), leaves less fuel unburnt and produces more energy. Exact mechanism, what triggers detonation, is not yet agreed upon. When originally proposed, Khokhlov (1991) assumed deflagration to detonation transition (DDT) at smaller densities (a few times $10^6$ g cm$^{-3}$, characteristic for distributed burning regime) as the most probable mechanism. DDT is observed in terrestrial chemical flames, however it is more problematic to explain it in unconstrained WD setting.

Different indirect mechanisms for triggering detonation were proposed over time, involving creation of extended regions with large temperature gradients by colliding masses of WD material with different velocities. Pulsating detonation scenario involves recollapse of the WD after deflagration phase in which not enough energy was released to unbind the star. The original implementation (see Hoeflich & Khokhlov (1996)) seems not plausible now, as accurately modeled 3D deflagration with central ignition does ordinarily produce enough energy to unbind a C+O WD, as reviewed in the previous subsection.

Asymmetric variations of this scenario, with slightly offcenter ignition, Gravitationally-Confined Detonation (GCD, Plewa et al. (2004)), Detonating Failed Deflagration Model (DFD, Plewa (2007)) do trigger detonations in 3D simulations. In these only a small fraction of fuel is burnt before the bubble driven by buoyancy breaks through WD surface, creating surface wave intensive enough to trigger detonation after colliding at diametrically opposite point of the WD surface. The main problem of these models is to get enough preexpansion before detonation so that significant amount of intermediate mass elements be produced, to agree with observations. Pre-expansion, depending on the mass burnt before the bubble breakthrough, strongly depends on the position of original ignition site. The problem is thus to propose some robust mechanism to rule out significantly offcenter ignitions. These models tend to overproduce iron-group elements in all simulations to date.

### 1.3 Simulations of deflagration phase

Here, after a brief overview of standard hydrodynamics, we describe flame-capturing (FC) technique (Khokhlov (1995)) used in SN Ia simulations for tracking flame position and prescribing heat release in artificially thickened (to be resolved in simulations) flame zone with intent to reproduce, on resolved scales, results of real, non-discretized, hydrodynamics. We then describe some problems of the original
implementation of FC found in this study, and outline topics presented in the thesis, mostly related to improving the FC model.

1.3.1 Hydrodynamics involved in simulations

Deflagration is described by a standard set of hydrodynamic equations with reaction source terms. These include a mass continuity equation; Navier-Stokes equation for velocity of the matter subject to gravity, pressure gradients and viscosity; transport equation for internal energy, with a source term describing heat release in reactions taking place in the system; and finally equations describing diffusion and reactions for species involved in reactions. Equations of state, expressing pressure and internal energy as functions of density and temperature make the system of equations closed. For SN Ia problem the system is usually simplified by neglecting viscosity and diffusion of species (as thermal conductivity by several orders of magnitude dominates other transfer phenomena: Prandtl number is small, Lewis number is large).

For large scale simulations the system is modified further: detailed reaction networks are not used, instead only a few species are taken into account, with model reaction rates for these, found separately in such a way that the reduced system imitated kinetics of the full system with acceptable accuracy. Such a simplification is used in chemical combustion simulations as well: this makes it possible to save computational resources, to be able to use higher resolution for example, when it is more important to resolve some critical hydrodynamic scales then to get exact distributions of species. This is usually the case in engineering applications, when, for example, knowing pressure or temperature distribution in combustion chamber is more important than knowing detailed chemistry of burning process.

In SN Ia problem using detailed reaction network in large-scale hydrodynamic simulations makes little sense in principle, as physical reaction zone (across which at least some species concentrations change significantly) is never resolved in such simulations, and this situation will not change in any foreseeable future. As the total simulation box size must be of the WD size, that is a few thousand kilometers, grid cells are of order 1 km size for most detailed of current simulations. Flame width is submillimeter for most of the deflagration (at density in front of the flame $\rho_{\text{fuel}} \sim 10^8$ g cm$^{-3}$ and above, Timmes & Woosley (1992)). Because of this disparity, all full star simulations evolve flame surface indirectly, without resolving flame width.

2. The latter is studied separately, for calibrating the reduced scheme in part, in simplified (usually steady 1D) setting, allowing to concentrate on kinetics rather than (trivial in such setup) aerodynamics.

3. The flame propagates directly on its own when the set of hydrodynamic equations described above is solved exactly. Then, as described in Sec. 1.2.2, interplay between heat release in the flame and heat conduction into cold material in front of the flame leads to flame propagating forward, with correct (by definition) speed. In simulations described in this paragraph, however, derivatives
One approach (level set method, LSM; used by Munich group in part, Reinecke et al. (2002a); Röpke et al. (2007)), motivated by tiny width of real flames, is to (formally) describe the flame as infinitely thin surface, on which matter density, velocity and other physical variables have hydrodynamically prescribed discontinuities. One then propagates this discontinuity surface with the speed prescribed so that to mimic, in average, real flame region evolution. This surface is represented as the zero-level of certain “level function” $G$: flame manifold $|t = \{ r(t) : G(r, t) = 0 \}$.

Time evolution of $G$ (advection plus normal propagation into the fuel with prescribed “flame” speed) used strives to ensure the needed evolution of the flame surface. Various numerical tricks are employed to take care of the tendency of $G$ to develop unphysical peculiarities. Hydrodynamical solvers (based on piecewise-parabolic reconstruction, Woodward & Colella (1984)) used in conjunction with this formally infinitely thin flame model spread discontinuities over several grid spacings, exact fractions of fuel/ash in grid cells intersected by the “flame surface” have more of numerical significance for the scheme than physical meaning.

We will stick to another flame-tracking prescription (described below), where the deflagration front is represented with artificial thick “flame”. Quotation marks are used below to distinguish the artificial numerical flame wherever confusion with real physical flame seems possible. We also refer to this numerical construction as “flame zone” as it is intended to be evolved in such a way so that to contain the physical flame within. The “flame” is governed by the same reaction-diffusion equations as physical flames, which makes it clear what behavior of the “flame” to expect (instabilities, interaction with background turbulence and sound waves), no new physics is introduced. This seems a clear advantage over LSM.

### 1.3.2 Flame capturing

Flame Capturing (FC) technique (Khokhlov (1995)) employs artificial scalar quantity $f(r,t) \in [0;1]$, “reaction progress variable”, to track flame evolution: $f = 0$ in the unburnt material, and changes to 1 behind the “flame”, when the burning is complete. The “flame” in the sense of this numerical technique is a region where $f$ is neither 0 nor 1 (but strictly between); it is made a few grid sizes thick by appropriately choosing parameters governing $f$ evolution (see below); the value of $1 - f$ is intended to mimic real physical fuel fraction in fuel/product mixture within the grid cell in the flame region.

are modeled via finite differences of quantities in adjacent grid cells. This modeling is designed to be accurate enough for fluid motions on scales exceeding a few grid spacings, yet obviously such differences cannot model derivatives of quantities changing significantly on subgrid scales, which is the case for reaction species abundances.

4. This in essence is a particular realization of artificial viscosity approach, Neumann & Richtmyer (1950).
\( f \) is evolved via a diffusion-type equation,
\[
\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f = \nabla (K \nabla f) + \Phi(f).
\] (1.3)

Physical quantities (pressure, temperature, composition, matter velocity) are simultaneously evolved through a standard system of Euler equation (5.2), diffusion-type equations with reaction terms for internal energy density (heat conduction equation) and species concentrations (if tracked separately; in standard FC realization they are just set to be a linear function of \( f \)), and equations of state (in code ALLA that we use for most non-steady simulations these are implemented as functions taking matter density and internal energy density as input, and returning pressure and temperature). \( f \) is coupled with physical variables through advection (by local matter velocity \( \mathbf{u} \) in (1.3)); and through heat-release term in hydrodynamic equations, which is governed directly by \( f \): \( \delta Q = q df \), that is heat is released linearly with \( f \) increasing (reaction progressing) up to \( q \), heat release of complete nuclear burning, per unit mass. (This \( q \) depends on local fuel composition and density.) Artificial diffusivity \( K \) and artificial “burning rate” \( \Phi(f) \) were prescribed (Khokhlov (1995)) so that to make the “flame” \( \sim 4 \Delta \) thick, \( \Delta \) denoting grid zone size, and propagating with prescribed velocity. That original prescription in effect led to systematic error in flame velocity, due to matter expansion (in the process of burning) neglected when estimating front speed in a system (1.3). This was corrected in Zhiglo (2007) (and will be described in the next chapter).

Scales larger than the flame width, which govern flame instabilities development (LD and RT), are not resolved in SN Ia simulations as well — for most of the simulation, at large densities; a portion of a flame within any grid cell is thus not smooth, but corrugated by instabilities. Real flame surface therefore exceeds the surface implied from numerical observations on grid scale. This is an extra complication, not encountered in shock-tracking techniques used similarly to FC in certain simulations with shocks. To address this issue all simulations include some subgrid model for prescribing renormalized, corrected for missing scales velocity, larger than physical laminar flame speed.

Observations of stationary RT-accelerated burning in Khokhlov (1995) led to using “turbulent flame speed” \( S_t \), defined through (1.1) where for \( \Delta \) the grid spacing is used, as the value for artificial “flame” propagation speed ensuring correct integral burning rate. When the laminar flame speed \( S_l \) exceeds \( S_t \), before developed RT-driven burning regime sets in, the “flame” is required to propagate with laminar speed \( S_l \). See Zhang et al. (2007) for further verification of this flame speed prescription, and for proposed technique modification in transient, non-stationary setting. We will

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5. Only constant \( K \) was used before Zhiglo (2007). Eq. 1.3 here is written in the form we use below with more general flame models, in which \( K \) is a function of \( f \).
not touch below on the best prescription for the “flame” speed, but concentrate on
the very model propagating the “flame” with a given speed.

1.3.3 Goals and scope of the thesis

To hope to get meaningful physical results in simulations it is critically important
to understand the properties of the model used for tracking the flame region and
for estimating heat release there. It is important that flame tracking model itself,
in part, did not introduce unphysical artifacts in uncontrolled way into simulations.
One needs to study model behavior in density range between $\sim 2 \times 10^9 \text{ g cm}^{-3}$ (cen-
tral WD density) and a few $\times 10^6 \text{ g cm}^{-3}$ (when distributed burning sets in, and
hypothetical deflagration to detonation transition could take place), and favor mod-
els not introducing much noise into simulations, and not demonstrating significant
instabilities of their own, unless there is a hope that the latter mimic instabilities of
actual physical flame zone.

When this work was started no analysis of features of the flame model used
for FC existed, apart from initial study of isotropy of “flame” propagation on the
grid in Khokhlov (1995), together with analytical estimates that led to prescription
for parameters in (1.3); the parameter values proposed there were used essentially
verbatim by several groups thereafter (Gamezo et al. (2003); Plewa et al. (2004);
Brown et al. (2005)). By now some results on numerical noises generated by flame
models, including description of a new burning rate proposed for use in FC, were
presented by our colleagues (Jordan et al. (2008)).

Numerical simulations always pose a question how reliable the results are, what
in the results is due to actual physics of the system studied, and what is an artifact
of the numerical scheme/approximation/model used. This question is particularly
important for systems so complex that simulations are the only way to get an es-
timate of the results. With these concerns results are always tested against other
simulations, with different resolution, utilizing different discretization algorithm or
based on analytically different solver. A suite of problems with known analytical
behavior is used to compare these known results with results of simulations, albeit
on simple systems. With all this care every so often discrepancies between results of
different groups appear. Khokhlov (1995) reports that 3-cell wide cylindrical flame
propagates isotropically on a square grid. Same FC model implemented by Niemeyer
required 8-cell wide flame to make anisotropies acceptable. GCD model reach robust
detonation conditions in 3D in FLASH group simulations (Jordan et al. (2008)), the
same model never detonates in simulations by Röpke et al. (2007). SN Ia simulations
in octant with central ignition show clear tendency of the flame to preferentially de-
velop features along grid directions from the very beginning of the simulation, which
is a clear numerical artifact (this further facilitates fast RT instability development).
Concerns like this were a part of motivation to study flame model features in detail.
In Chap. 2 we present results obtained mostly without using actual non-steady hydrodynamical solvers. We describe a method we developed for finding flame speed by solving eigenvalue steady-state problem. We use that method to calibrate the model flame used in Khokhlov (1995) for flame capturing. In original calibration in Khokhlov (1995) matter expansion (we characterize it with expansion parameter $\Lambda = \rho_{\text{ash}} / (\rho_{\text{fuel}} - \rho_{\text{ash}})$) in a result of burning was neglected; we correct for this and propose additional improvement, allowing to keep flame width independent of matter expansion (this expansion increases with fuel density decreasing, due to decreasing degeneracy of the electron gas). We present analytical solution for the original model flame profiles, which allows us to directly check the eigenvalue numerical scheme. Flame profile (distribution of $f$ in space for a steadily propagating flame solution of (1.3)) has an exponential tail; we propose another class of models, with $f$-dependent diffusivity coefficients, that produce flames localized in space (having finite total width, with no tails). We argue about the advantages of models having such finite flames, and find certain representative model of that class with nearly linear flame profiles (similar in that to real fuel distribution in shaped with RT-instability flame zone in simulations of SN Ia), which are furthermore insensitive to $\Lambda$. For this model we present simple fits of the the parameters entering (1.3) as functions of $\Lambda$, yielding very simple implementation of the new model proposed in flame capturing numerical scheme. We conclude Chap. 2 by presenting results of actual implementation in FC technique, observed flame speeds, widths and profiles. Discrepancy with steady-state results are clearly connected to discretization effects by varying resolution, number of cells within the flame width.

Chap. 3 is devoted to studying noises produced by FC scheme in 1D simulations. Two new quiet models are introduced, that have finite flame widths and unique eigenvalues for flame speeds. They are calibrated to yield correct "flame" speeds and widths using the methods of Chap. 2.

In Chap. 4 we study 2D and 3D behavior of model flames. By modeling circular flames in 2D we observe that anisotropic propagation speed is a generic feature of reaction-diffusion flames, more prominent at higher expansions. This is a purely numerical effect, and is cured by increasing flame width. For one of the new quiet flame models, sKPP, this effect is especially pronounced: for flame width of about 8 cells between reaction progress variable values $f = 0.01$ and $f = 0.99$ the flame propagates along grid axes by $> 5\%$ faster than at 45 degrees to them, for expansions corresponding to deflagration in WD at relevant densities of $10^8 \text{ g cm}^{-3}$ and below. A free parameter of the second of the quiet models of Chap. 3 is used to eliminate propagation anisotropy at all relevant expansions. We observe LD instability, particularly severe for sKPP model of Chap. 3 at larger expansions. These 2D effects are a strong argument to avoid using sKPP model at densities of $\lesssim 10^8 \text{ g cm}^{-3}$. Second of the quiet models, model B, shows significantly larger critical LD wavelength, and slower growth of this instability. At all densities above $3 \times 10^7 \text{ g cm}^{-3}$ in SN Ia
problem maximal combined 2D asphericity due to both LD and numerical effects stays within 1.2% for simulation times exceeding those used in SN Ia simulations. At lower densities, and in 3D simulations, combined asphericity is larger yet tolerable for the “flame” width used, about 5.5–6 cells between \( f = 0.01 \) and \( f = 0.99 \), which is thinner than in original model of Khokhlov (1995)\(^6\). We present simulations of perturbed planar flames in 2D; observed critical wavelengths for perturbations to grow agree with theoretical \( \lambda_{cr} \) for LD instability (in Markstein approximation of infinitely thin flame with curvature-dependent propagation speed).

We develop quasi-steady technique for estimating Markstein numbers \( M \) (quantifying flame speed dependence on flame curvature for curved multidimensional flames) in Chap. 5, and calculate these for models described in the thesis. \( \lambda_{cr} \) for LD instability depends on \( M \). Comparison with \( \lambda_{cr} \) estimated directly in Chap. 4, as well as comparisons of exact \( M \) found here with \( M \)'s estimated numerically provides evidence that Model B is well-understood, and in its observed behavior physical effects dominate over numerical ones.

We conclude that model B proposed here is best suited for use for Flame Capturing.

\(^6\) The thinner the “flame” is the better for resolving its small scale features, ultimately for better accuracy of the simulation.
CHAPTER 2
STEADY STATE ANALYSIS OF 1D FLAMES

In the present chapter we decouple equation for reaction progress variable $f$ in (1.3) from the rest of hydrodynamic equations, and study its flame-like solutions in steady 1D setting. We write a master equation for steady flame profile $f(x)$ in dimensionless form, and find dimensionless velocities $d$ and widths $w$ for a few artificial burning rates $\Phi(f)$ used in combustion literature, as well as, in Sec. 2.4, for nonconstant diffusivity $K(f)$ proposed during this work. Accuracy of the numerical scheme proposed for finding $d$ and $w$ is tested against analytic results obtained for one model (original one, Khokhlov (1995)) and qualitative results for another one, KPP. Restoring normalization of the master equation (2.2) leads to a simple prescription for choosing scale-factors $R$ and $\tilde{K}$ of reaction rate and diffusivity, such that the flame with coefficients (2.7) will propagate with prescribed speed $D$ and have prescribed width $W$, for any expansion $\Lambda$. These scalings (2.37) are determined based on dimensionless $d(\Lambda), w(\Lambda)$ found in the first sections of this chapter and fitted in Sec. 2.5 for efficient numerical implementation. In the last section we check our results in practice, in ALLA code.

Methods for calibrating flame models presented in this chapter are used for different models in the rest of the thesis; qualitative results for various possible burning rates are used for constructing a new flame model (Model B) in the next chapter, which we ultimately suggest for use in FC based on properties of the “flames” it produces; eigenvalue problem used in this chapter for finding $d$ and getting flame profiles is generalized in Chap. 5 for spherical flames in higher-dimensional problems, to study effects of curvature on flames.

2.1 Physical formulation and numerical method

Here we study time evolution of the reaction progress variable profile $f(r)$, which determines heat release in hydrodynamic simulations. In 1D it is possible to decouple equation (1.3) for $f$ from the rest of hydrodynamic equations for any equations of state — provided the burning rate can be considered depending on $f$ only. This is the case for 1 stage reactions when $Le = 1$ (when temperature and reactant concentration distributions are similar, Zeldovich & Frank-Kamenetskii (1938); relevant for terrestrial chemical flames), and for FC progress variable $f$, by construction. Here we demonstrate this decoupling, formulate the steady-state problem and describe numerical procedure we use for its solution.
2.1.1 Boundary problem for flame speed

All models studied in this chapter are of form (1.3). One particular type of solutions of (1.3) coupled to hydrodynamic equations (as well as of real combustion systems) in homogeneous medium is steady 1D flame front, propagating with constant speed $D_f$ into the fuel ($D_f$ is defined here as the speed of the flame in the reference frame where the fuel rests). Here we study these particular 1D solutions, with physical quantities (and $f$) being functions of $x - D_f t$ only. In such a steady solution it is convenient to study the system in a flame rest-frame, in which all physical quantities depend on $x$ only (after Galilean transformation). Matter velocity (in this 1D steady setting) is determined by continuity equation:

$$u(x)\rho(x) = \text{const} = -D_f \rho_0.$$  

(2.1)

This further determines $f(x)$ from (1.3), which after this substitution for $u(x)$ reads

$$-D_f \frac{\rho_0}{\rho(x)} \frac{df}{dx} = \frac{d}{dx} \left( \frac{K df}{dx} \right) + \Phi(f).$$

(2.2)

To close the system one needs to express $\rho(x)$ via heat release distribution, $dQ/dx = q df/dx$. For this, in isobaric burning, one determines $\rho(x)$ from enthalpy conservation,

$$H(p_0, \rho_0) + qf = H(p_0, \rho),$$

which in particular provides $\rho_0/\rho(x)$ as a function of $f$ (depending on the particular equation of state). This makes (2.2) a second order equation for $f$ only.

In certain physically interesting situations, e.g. near the center of a WD (main contribution to pressure from ultrarelativistic degenerate electron gas), or for ideal gas (terrestrial flames) $\rho \propto 1/H$ at constant pressure\(^1\), thus (2.2) assumes the following form,

$$-D_f \left( 1 + \frac{f}{\Lambda} \right) \frac{df}{dx} = \frac{d}{dx} \left( \frac{K df}{dx} \right) + \Phi(f),$$

(2.3)

which we use for steady-state flame speed and width estimates.

$$\Lambda = \frac{\rho_{\text{ash}}}{\rho_{\text{fuel}} - \rho_{\text{ash}}}$$

(2.4)

quantifies how the matter expands as a result of burning; with $\Lambda$ defined this way eigenvalues found from (2.3) are close to true ones even for situations with $H \rho$ slightly

\(^1\) this generally is the case for “$\gamma$ equation of state”, $H = \frac{\gamma p}{\gamma - 1}$ (for ideal gases this is the case when specific heat is independent of temperature.)
nonconstant across the flame. $\Lambda = \gamma - 1 \frac{P_0}{q_0}$ for ideal gas equation of state, $\gamma$ denoting adiabatic parameter ($\gamma = c_p/c_v$ for ideal gas).

For solution $f(x)$ to describe a physically meaningful flame profile it needs to satisfy physical boundary conditions,

\[
\begin{align*}
  f(-\infty) &= 1 \\
  f(+\infty) &= 0.
\end{align*}
\]  

These may be satisfied only for certain values of $D_f$ (a parameter in (2.2)); these eigenvalues of $D_f$ are by definition possible flame propagation speeds in 1D. Corresponding eigenfunctions, $f(x)$ satisfying (2.3–2.6), are steady flame profiles; in flame capturing these will determine “flame” thickness and fuel distribution within the “flame” — approximately, as long as the “flame” segment propagation may be treated as 1D steady-state, and up to discrepancies due to numerical (discretization) effects.

2.1.2 Numerical procedure

First, by representing burning rate and diffusivity as products of constant dimensionful scale-factors and ($f$-dependent in general) dimensionless form-factors,

\[
\Phi(f) = R\Phi_0(f), \quad K(f) = \tilde{K}K_0(f)
\]

we rewrite (2.3) in dimensionless form:

\[
-d \left( 1 + \frac{f}{\Lambda} \right) \frac{df}{d\chi} = \frac{d}{d\chi} \left( \frac{K_0(f)df}{d\chi} \right) + \Phi_0(f). \tag{2.8}
\]

To accomplish this we have introduced dimensionless flame speed,

\[
d = D_f/\sqrt{\tilde{K}R}, \tag{2.9}
\]

and dimensionless coordinate

\[
\chi = x\sqrt{R/\tilde{K}}
\]

along flame propagation. Eigenvalue $d$ of boundary value problem (2.8) with boundary conditions following from (2.5–2.6) may be found numerically following the procedure described next (see Zhiglo (2007) for more detail).

As (2.8) is invariant under translations in $\chi$ it can generically be reduced to a first order equation by rewriting it in terms of

\[
p = -\frac{df}{d\chi}
\]
considered a function of $f$:

$$\frac{d}{df}(K_0(f)p) - d\left(1 + \frac{f}{\Lambda}\right) + \frac{\Phi_0(f)}{p} = 0 \quad (2.10)$$

This form is used below for qualitative and numerical analysis of the problem. Corresponding boundary conditions are $p(0) = p(1) = 0$. Eigenfunctions $p(f)$ are non-negative.

In this section we demonstrate the technique for systems with constant diffusivity: the original model of Khokhlov (1995) ($f_0 = 0.3$ used there) with step-function rate

$$\Phi = \begin{cases} R & \text{for } f_0 < f < 1 \\ 0 & \text{otherwise} \end{cases} \quad (2.11)$$

and KPP (Kolmogorov et al. (1937))

$$\Phi = R f (1 - f) \quad (\text{for } 0 < f < 1). \quad (2.12)$$

Equation (2.10) is integrated by the fourth order Runge-Kutta algorithm starting from $f = 1$, $p = 0$. We use constant grid spacing ($\Delta f = 10^{-5}$ for most of the runs), except near zeroes of $p$ (the starting point $p(f = 1) = 0$, and at most one more), where it was refined further.

Integration is actually started at $f_\delta = 1 - \delta$, with $\delta$ being the smallest refined integration step, as $p(f = 1) = 0$ appears in the denominator of (2.10). Analytically found asymptotic expansion is used as initial value for $p(f_\delta)$ (see Chap. 5 for more details in more complicated setting in $D > 1$ dimensions. Using $\alpha = D - 1 = 0$ in Eq. 5.18, and similar equations below that for $p$ for different flame models, yields asymptotics valid for 1D flames.)

The $d$ eigenvalue is then found for step-function $\Phi_0(f)$ by requiring $p|_{f=1} = 0$. Namely, Newton-Raphson algorithm (see, e.g. Press et al. (1992)) is applied, $\frac{\partial (p(f=1))}{\partial d}$ is found simultaneously with $p(f)$, ensuring fast convergence. $d(\Lambda = \infty)$ (found beforehand by solving (2.18)) is used as a seed at each new $f_0$ value for the first $\Lambda$ in a row; for subsequent $\Lambda$’s the previous one provides seed value for $d$; 4–13 iterations were enough to get $d$ with $10^{-8}$ precision. Results are summarized in Sec. 5.1. For the case of KPP burning rate the spectrum of steady flame speeds is actually continuous, as for the studied (Kolmogorov et al. (1937)) case with no matter expansion. We explain qualitatively this feature of the spectrum in the next section.

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2. It is imperative to start from $f = 1$ for parabolic $\Phi_0(f)$ (KPP) as a general solution for $f(x)$ near $x \to +\infty$ (where $f \to 0$) is a superposition of two decaying exponentials, and the faster decaying one is lost when integrating $dp/df$, thus making it impossible to satisfy $p|_{f=1} = 0$. 
2.2 Spectrum of flame speeds and flame profiles. Qualitative and numerical analysis

Here we show qualitatively why an eigenproblem with step-function burning rate has unique solution for $D_f$ but the problem based on KPP has continuous spectrum of eigenvalues. We describe asymptotic behavior of flame profiles near $f = 0$ and $1$, to better understand physical versus numerical features of 1D non-steady simulated “flame” in Sec. 2.6, and, with this understanding, to propose new flame models in Sec. 3.1. Qualitative consideration is confirmed by numerically solving the eigenproblem for $d$, and by numerical integration of (2.10) for several $d$'s.

2.2.1 Step-function burning rate

We start with the model described by (2.8) with step-function burning rate (2.11). One can observe that an eigenfunction $f(\chi)$ is monotonically decreasing, in accord with physical expectations (see typical flame profiles in Fig. 2.1). More than that, $f(x)$ is convex at $f < f_0$ and concave elsewhere. Really, the solution of (2.10) at $f < f_0$ is $p = df(1 + f/2\Lambda)$, positive and increasing. It is thus enough to show that $p$ is monotonically decreasing in $(f_0; 1)$ (then $p$ is automatically positive as it goes to 0 at $f \to 1$ as dictated by the boundary conditions). If $p$ were not decreasing there would have existed $f_r \in (f_0; 1)$ such that $dp/df(f_r) = 0$. By (2.10) $p(f_r) = (d(1 + f_r/\Lambda))^{-1}$, $d^2p/df^2(f_r) = d/\Lambda > 0$, thus $p$ would have been increasing in some right neighborhood of $f_r$, and then (2.10) would require that $p$ grew on entire $(f_0; 1)$, making $p(f = 1) = 0$ impossible.

Any self-similar solution satisfying physical boundary conditions must behave as follows (for certain $\chi_1$):

$$f = 1 \forall \chi < \chi_1, \quad df/d\chi(\chi_1) = 0, \quad 0 < f < 1 \text{ at } \chi > \chi_1, \quad \lim_{\chi \to -\infty} f(\chi) = 0. \quad (2.13)$$

Really, any solution of (2.10) equal to 1 at any point with non-zero $df/d\chi$ would necessarily exceed 1 nearby. While we could allow systems with profiles $f$ taking values outside $[0; 1]$, for our particular model with rate $\Phi(f) = 0$ at $f \geq 1$ any solution exceeding $f = 1$ at some $\chi$ monotonically goes to $+\infty$ to the left of such a $\chi$, as $\chi \to -\infty$ (so the boundary conditions are not satisfied). Thus $f$ must either become identically 1 on some half-line $(-\infty; \chi_1]$ or approach $f = 1$ asymptotically from below as $\chi \to -\infty$. Behavior of the solution of (2.10) in the region where $|1 - f| \ll 1$ coincides with that of the linearized equation,

$$f = \bar{c}_1 - \chi/\bar{d} + \bar{c}_2 \exp(-\bar{d}\chi), \quad (2.14)$$
where
\[ \bar{d} = d \left( 1 + \frac{1}{\Lambda} \right). \quad (2.15) \]
The latter does not remain in the vicinity of 1 as \( \chi \to -\infty \) (in fact is unbounded) for any values of integration constants \( \bar{c}_{1,2} \), unless it is differentiably glued to the \( f = 1 \) solution to the left of some \( \chi_1 \). This completes the proof for the behavior near \( f = 1 \).

Similar analysis in the region where \( |f| \ll 1 \) yields a general solution of the linearized equation
\[ f = c_1 + c_2 \exp(-d\chi), \quad (2.16) \]
which tends to 0 at \( \chi \to -\infty \) if and only if \( c_1 = 0 \). From this it follows that any solution of (2.10) such that \( f(\infty) = 0 \) cannot equal zero at any finite point. It has an infinite tail, decaying exponentially.

Figure 2.1: Flame profiles (i.e. numerically found eigenfunctions). For each \( f_0 \) (the ordinate of the curve intersection with \( \chi = 0 \)) 3 pairs of profiles are depicted, for \( 1/\Lambda = 0.05, 4, \) and 20, larger \( 1/\Lambda \) corresponding to the curves intersecting \( \chi = 0 \) axis at larger angles.

Summing up, the desired eigenfunction asymptotically behaves like (2.16) with \( c_1 = 0 \) as \( \chi \to +\infty \), and like (2.14) as \( \chi \to \chi_1 + (\chi_1 = x_1 \sqrt{R/K}) \), with \( \bar{c}_{1,2} \) such that
\[ f(\chi_1) = 1, \; df/d\chi(\chi_1) = 0. \quad (2.17) \]
For any fixed \( \chi_1 \) a solution \( f_{\chi_1} \) satisfying (2.17) is unique, and any solution with \( f(-\infty) = 1 \) is a translation of such. In order for this \( f \) to vanish at \( +\infty \) it must belong to another one-parameter subset of solutions. For this to happen there must
be one functional dependence among the parameters in (2.10). As it is shown below, this actually leads to a unique value for \( d \) for any fixed values of the other parameters (\( \Lambda \) and \( f_0 \) here), for which solutions of the boundary problem exist.

In the \( q = 0 \) (\( \Rightarrow \rho(x) = \rho_0 = \text{const} \)) case (2.10) actually is piecewise linear, thus the above restrictions immediately yield \( d(\Lambda = \infty, f_0) \) as the solution of equation

\[
f_0d^2 = 1 - e^{-d^2}.
\]

(Cf. (2.26); \( f(\chi_1) \) is then expressed in elementary functions as \( \Lambda = \infty \)). One can write the solution as expansion in \( f_0 \) asymptotically as \( d^2 = \frac{1}{f_0} - \frac{e^{-1/f_0}}{f_0} - \frac{e^{-2/f_0}}{f_0^2} - \left( \frac{3}{2f_0^2} + \frac{2}{f_0} + \frac{2}{f_0^2} \right) e^{-3/f_0} + O \left( (f_0 e^{1/f_0})^{-4} \right) \); at \( f_0 = 0.3 \) this yields \( d \) 2% smaller than the value in Khokhlov (1995) (where in \( q = 0 \) approximation \( f(x) \) was found incorrectly); at \( \Lambda \)'s of interest the difference will be more significant. In the limit \( f_0 \to 1 \) \( d \) vanishes as \( d^2 = 2(1 - f_0) + \frac{2}{3}(1 - f_0)^2 + \frac{7}{9}(1 - f_0)^3 + \ldots \) (leading term agreeing with an estimate in Zeldovich et al. (1985), p. 266).

Flame profiles found numerically using the procedure described in the previous section are presented in Fig. 2.1. They demonstrate asymptotic behavior as found above, and show how the profile width depends on expansion parameter \( \Lambda \).

### 2.2.2 KPP burning rate

It is known (see Zeldovich et al. (1985) for detailed discussion) that the spectrum of eigenvalues of KPP problem is continuous, comprising all reals above some \( d_1 \). In this section we show that the same holds if one includes the term arising from gas expansion, find similar spectrum for a wide range of \( \Phi \)'s and verify these conclusions numerically.

One can qualitatively analyze the spectrum for burning rate (2.12) along the same lines as for (2.11) described in the previous section. Upon linearization in the region where \( 1 - f \ll 1 \) (\( \chi \to -\infty \)) (2.8) yields

\[
f = 1 - b_+ e^{-\tilde{\lambda}+\chi} - b_- e^{-\tilde{\lambda}-\chi}, \quad \tilde{\lambda}_{\pm} = \frac{d}{2} \pm \sqrt{\frac{d^2}{4} + 1},
\]

\( \tilde{d} = d(1 + 1/\Lambda) \) as before; thus there is a one parameter subset of physical solutions, those behaving asymptotically like (2.19) with \( b_+ = 0 \).

By linearizing (2.8) in the region where \( f \ll 1 \) one gets asymptotic behavior of a solution

\[
f \approx b_+ e^{-\lambda+\chi} + b_- e^{-\lambda-\chi}, \quad \lambda_{\pm} = \frac{d}{2} \pm \sqrt{\frac{d^2}{4} - 1}.
\]
There are a priori three different situations for drawing further conclusions:

1) $d < 2$: any solution getting to a neighborhood of 0 necessarily becomes negative.

2) $d > 2$: any $b_+, b_- \geq 0$ describe physically acceptable behavior, as does a certain subset of $b_+ < 0$, $b_- > 0$. Thus one may conjecture that for all $d > 2$ there is an eigenfunction: it belongs to the described above 1-parameter subset of solutions asymptotically approaching 1 as $\chi \to -\infty$ and on becoming small at larger $\chi$ it behaves asymptotically like (2.20), exponentially approaching zero as $\chi \to +\infty$. The resulting 1-parameter set of physical solutions corresponds to one of them translated arbitrarily along $\chi$, i.e. there is a unique flame profile for any $d$ (the term “unique” as related to profiles is used below in this sense, i.e. up to translations).

By analyzing (2.8) one expects the $f$ to decrease monotonically, and it is easy to see that a solution cannot asymptotically approach any value in $(0; 1)$ as $x \to +\infty$ (say, by linearizing (2.8) near such a value). Thus a solution will eventually get to a neighborhood of $f = 0$, where it will behave as (2.20); unless it becomes negative (i.e. have unphysical $b_\pm$, $b_- < 0$ in part; numerical results below show that this does not happen, as well as confirm the form of the flame profile) it will asymptotically go to zero, hence being physical. It is the presence of 2-parameter set of solutions decaying to zero at $\chi \to +\infty$ which accounts for the continuous spectrum of $d$ here, in contrast with the situation with step-function burning rate.

To compare side-by-side one may start with some physical (satisfying $f(\chi = -\infty) = 1$) $f$ on the left and check if it can satisfy $f(\chi = +\infty) = 0$ as well. For step-function there is a unique solution (modulo translations) which goes to zero as $\chi \to +\infty$. Other solutions asymptotically approach non-zero values; a solution asymptotically approaching some $c_1 < f_0$ reads

$$f(\chi > 0) = c_1 + 2\Lambda \left(1 + \frac{2\Lambda}{f_0 - c_1}\right)e^{d(1 + \frac{c_1}{f_0})\chi - 1}$$

(2.21)

(up to translations in $\chi$). As $c_1$ increases from 0 to $f_0$ derivative $\frac{df}{d\chi}|_{f=f_0}$ increases monotonically from $-f_0d\left(\frac{f_0}{2\Lambda} + 1\right)$ to 0. If for a given $d$ the (unique up to translations) $f$ going to 1 as $\chi \to -\infty$ has $\frac{df}{d\chi}|_{f=f_0} \in [-f_0d(\frac{f_0}{2\Lambda} + 1); 0]$ it will go asymptotically to the corresponding $c_1$ as $\chi \to +\infty$, namely it will be exactly (2.21) where $f < f_0$; if its derivative is more negative, it will be described by (2.21) with negative $c_1$ until it intersects $f = 0$ at some finite $\chi$ (and this is not a solution we are interested in). Easily established monotonousness properties (how the slope $\frac{df}{d\chi}|_{f=f_0}$ varies with $d$) prove this way the claim that there is a unique $d$ for which the physical solution (according to its behavior near $f = 1$) goes asymptotically to zero as
\( \chi \to -\infty \). For the \( \Phi(f) \) (2.12), on the other hand, there are no solutions going asymptotically to any constant but 0 as \( \chi \to +\infty \), but those going to 0 represent a two-parameter set of solutions, and depending on the \( b_\pm \) in their asymptote the \( \left. \frac{df}{d\chi} \right|_{f=f_0} \) may take different values, thus making it possible to match this slope of the solution physical near \( f = 1 \) for a range of \( d \)'s. (In this case \( f_0 \) denotes some intermediate value of \( f \), between 0 and 1.)

3) \( d = 2 \): asymptotic solution (2.20) must be rewritten as \( f(\chi) = (b + b_0 \chi) e^{-\frac{d}{2} \chi} \), and there is again a 2D domain of physical \((b, b_0)\), yielding \( f > 0 \), \( f \to 0 \) as \( \chi \to +\infty \). In this case a meaningful burning profile exists as well.

|  \hline | \hline |
|---|---|
| \( d = 1 \) | \( d = 2 \) |
| \( d = 5 \) | \( d = 20 \) |

Figure 2.2: KPP flame profiles at different \( \Lambda \) and \( d \). For each \( d \) 3 curves are depicted, for \( 1/\Lambda = 0.05, 5, \) and 20, larger \( 1/\Lambda \) corresponding to the curves intersecting \( \chi = 0 \) axis (where \( f \) was set to 0.5) at larger angles, and having larger widths.

Flame profiles \( f(\chi) \) found numerically for \( \Phi_0(f) = f(1-f) \) are shown in Fig. 2.2 for four values of \( d \). These seem to satisfy the boundary conditions for \( d \geq 2 \), whereas the profiles for \( d = 1 \) (each integrated from \( p(1) \equiv -df/d\chi|_{f=1} = 0 \)) intersect \( f = 0 \) at finite \( \chi \) with non-zero \( df/d\chi \). Corresponding integral curves \( p(f) \) at the same values of \( d \) and \( \Lambda \) are presented in Fig. 2.3. Note that for \( d = 1 \) \( p|_{f=0} \neq 0 \), whereas for \( d \geq 2 \) it was checked that by refining the grid \( p(0) \) became correspondingly closer to 0, down to \( p(0) \approx 10^{-10} \) at the bulk grid spacing of \( 10^{-7} \) (at finer grid rounding errors in double precision reals dominated). This numerically confirms our qualitative conclusions about continuous spectrum \([2; \infty)\) for \( d \) in KPP model.

One can observe that the flame width grows fast with \( d \). As in the original model (Kolmogorov et al. (1937)) one may conclude that only propagation with
the smallest velocity is stable (only asymptotes near \( f = 0 \) are essential for the argument to hold, and these have the same exponential form regardless of \( \Lambda \)). Of course, if the \( f(x) \) at some time corresponds to some eigenfunction above, such a profile will propagate with corresponding \( d \). But if one considers a process of setting up the steady-state propagation, with initial \( f(x) \) corresponding to pure fuel on a half-line (or \( f \) decaying with \( x \) faster than the fastest exponent \( \lambda_{-}(d = 2) = 1 \) in (2.20)) the resulting self-similar front will be the eigenvector with the smallest velocity. More generally, by considering the evolution of some superposition \( \Psi \) of the steady-state profiles found above one concludes that amplitudes of all of them but one will (asymptotically) decrease in time in favor of the one with the smallest \( d \) in the spectrum of \( \Psi \) (they interact due to nonlinearity of the system). As a generic perturbation is a superposition of all eigenfunctions, however small it is it will eventually reshuffle the profile into that for smallest \( d \).

Figure 2.3: Slope \( p(f) \) of the profile of KPP flame, integrated from \( f = 1, p = 0 \) at \( \Lambda \) and \( d \) as in Fig. 2.2; larger \( 1/\Lambda \) correspond to smaller \( p \). Note that at \( d = 1 \) \( p(f = 0) \) is non-zero, in contrast with the \( d \geq 2 \) curves.

2.2.3 General burning rate

Observations above may be extended for more general burning rate function as follows:

i) If \( \Phi_{0}(f) \) goes to some positive constant as \( f \to 0 \) there are no solutions going to 0 as \( x \to +\infty \). From a physical viewpoint a system reacting with finite rate in the initial state is unstable and self-similar solutions cannot exist. Problems with
Φ₀(0+) = ν < 0 do have eigenvalues (discrete spectrum). Corresponding eigenfunctions are identically zero on the right of some χ₂. \( f = -ν(χ - χ₂)^2/2 + O((χ - χ₂)^3) \) as \( χ \to χ₂^- \). sKPP model studied in the next chapter is of this type.

ii) For \( Φ₀(f) = μf + o(f) \) at \( f \to 0 \) non-negative solutions going to 0 as \( x \to +\infty \) exist iff \( d \geq 2\sqrt{μ} \), \( μ > 0 \) for \( Φ₀(f) \) to be positive (what is usually assumed in literature. See below for \( μ < 0 \) case). General solution getting to a vicinity of \( f = 0 \) decays exponentially. Analysis near \( f = 1 \iff \tilde{f} = 1 - f \ll 1 \) then suggests the following for \( Φ₀ = \tilde{ν} + \tilde{μ}\tilde{f} + o(\tilde{f}) \) (below \( d \geq 2\sqrt{μ} \) is assumed; \( f(−∞) = 1 \) required):

- \( \tilde{ν} > 0, \tilde{μ} > 0 \) — for all \( d \) (the above \( d \geq 2\sqrt{μ} \) assumed) a unique profile exists and \( \exists x₁ : ∀x < x₁ f(x) ≡ 1 \).
- \( \tilde{ν} > 0, \tilde{μ} \leq 0 \) — a unique profile whenever \( \tilde{d} ≡ d(1 + \frac{1}{\Lambda}) \geq 2\sqrt{-\tilde{μ}} \) (i.e. for \( |\tilde{μ}| > μ(1 + 1/Λ)^2 \) the spectrum is additionally shrunk); again identically 1 on a half-line. For \( \tilde{d} < 2\sqrt{-\tilde{μ}} \) there may exist solutions oscillating around \( f = 1 \), glued to \( f = 1 \) on some \((-∞; x₁) \). These violate \( 0 ≤ f ≤ 1 \), yet may be used in FC in principle. Besides, \( f(x₁+) < 1 \) and there may exist situations when \( f \) does not exceed 1 anywhere.
- \( \tilde{ν} < 0 \) — no physical solutions. For \( \tilde{μ} < 0 \) and \( \tilde{d} < 2\sqrt{-\tilde{μ}} \) there may be solutions glued to \( f = 1 \) on some \((-∞; x₁) \), but necessarily \( f(x₁+) > 1 \).
- \( \tilde{ν} = 0, \tilde{μ} > 0 \) — a unique solution exponentially approaching 1 as \( x \to −∞ \) \( ∀d \).

No physical solutions if \( \tilde{μ} < 0 \).

- \( \tilde{ν} = \tilde{μ} = 0 \). If \( Φ₀(f) = \tilde{q}\tilde{f}^\tilde{r} + o(\tilde{f}^\tilde{r}) \), \( \tilde{r} > 1 \), \( ∀d \) a unique solution exists. The solution of (2.10) may be written as \( p = \frac{\tilde{q}}{\tilde{d}}\tilde{f}^{\tilde{r}}(1 + \frac{\tilde{f}}{\chi_\Lambda} - \frac{\tilde{r} - 1}{\tilde{d}^\tilde{r}}\tilde{f}^{\tilde{r} - 1} + O(\tilde{f}^2 + \tilde{f}^\tilde{r})) \), leading to \( \tilde{f} \sim ((1 - \tilde{r})\tilde{q}\chi/\tilde{d})^{\frac{1}{2 - \tilde{r}}} (\tilde{q} > 0 \text{ assumed}) \). If \( Φ₀(f) \equiv 0 \) in some neighborhood of \( f = 1 \) bounded solutions exist but \( f \to 1 \) at \( x \to −∞ \) \( \text{from above} \). Again, usable in principle even though \( f(χ) \) is not monotonic.

- \( Φ₀ \sim \tilde{q}\tilde{f}^\tilde{r} \), but \( \tilde{r} \in (0; 1) \). \( \tilde{f} \) vanishes identically on the left of some \( χ₁ \), in its right neighborhood \( \tilde{f} \sim (\sqrt{\tilde{q}/2(1 + \tilde{r})})(1 - \tilde{r})(\chi - χ₁)^{\frac{t}{2 - \tilde{r}}} \).

iii) \( Φ₀(f) = μf + o(f), μ < 0 \) (⇒ \( Φ₀(f) < 0 \) near \( f = 0 \)). For any \( d \) a unique profile with \( f(+\infty) = 0 \), exponentially approaching. Behavior near \( f = 1 \) is described as in ii), depending on \( Φ₀(f → 1−) \), but because of the unique profile physical near \( f = 0 \) the spectrum of \( d \) is discrete (or empty).

iv) For \( Φ₀(f) = qf^r \) near \( f = 0 \) \( q > 0 \) there are no solutions of (2.10) with \( p(+0) = 0 \) when \( r < 1 \) — a situation analogous to i). As a further analogy, when \( q < 0 \) there may be a solution (unique up to translations); for this \( \exists x₂ : f = 0 \) at \( x > x₂ \), \( f(x → x₂−) \approx \left((x₂ - x)(1 - r)\sqrt{-q/(2(r + 1))}\right)^{\frac{2}{2 - r}} \). Using \( r = 0 \) here yields corresponding behavior in i). When \( r > 1 \) on the other hand, there are multiple solutions going to 0 (the ODE’s peculiarity; general solution decays as \( f \approx ((r - 1)qx/d)^{1/(1 - r)} \), hence one expects the same behavior as in ii) (apart from this power-law tail into fuel), depending on the \( Φ₀ \) shape near \( f = 1 \). When
\( \Phi_0(f) \equiv 0 \) in some neighborhood of \( f = 0 \) one expects a discrete spectrum of \( d \), with corresponding eigenfunctions behaving near \( f = 1 \) according to the \( \Phi_0(f) \) near 1, as in ii).

Summing this up, KPP-like behavior is quite universal for \( \Phi_0(f) \) going to 0 linearly or faster at \( f \to 0 \). \( \Phi_0(f) \equiv 0 \) near \( f = 0 \) leads to discrete spectrum; positive \( \Phi_0(f) \) decreasing slower than linearly (or not going to zero) as \( f \to 0 \) leads to absence of steady-state solutions. Eigenfunction \( f(x) \) has an infinite tail at \( f = 1 \) if \( \Phi_0|_{f\to1} \) decreases linearly or faster.

It should be stressed that these conclusions are based on analysis of asymptotic behavior of solutions near \( f = 0 \) or 1; as with KPP case considered above the fact that there is a 2-parameter set of solutions going to zero as \( f \to 0 \), say, is not enough to make claims as to global behavior of a solution physical near 1 — it may still become negative or unbounded near 0. For the cases with claimed continuous spectrum of eigenvalues the way the second term in (2.10) damps the solution near \( f = 0 \) suggests that for any fixed \( \Lambda \) the spectrum contains all reals above some \( d_\Lambda \). Some estimates of this lowest eigenvalue (for the case without expansion), and references can be found in Xin (2000) (I am grateful to Lenya Ryzhik for pointing out this review to me). Numerical studies of several models (with \((r, \tilde{r}) = (2,1); (5,1); (0.5,1); (1,2); (1,0.5)\)) agree with general claims of previous paragraphs. A new element appears (in contrast to KPP) for more general power law decay of the burning rate near \( f = 1 \) and \( f = 0 \): the lower boundary of eigenvalues \( d_\Lambda \) may depend on \( \Lambda \). Say, for \( \Phi_0 = f^2(1-f) \) it was observed that \( d = 1 \) was an eigenvalue for \( 1/\Lambda = \{0.05; 4; 20\} \); \( d = 0.464 \) was an eigenvalue for \( 1/\Lambda = \{4; 20\} \) but not 0.05; and \( d = 0.215 \) was an eigenvalue for \( 1/\Lambda = 20 \) but not 4 or 0.05. Asymptotic behavior of solutions near \( f = 0 \) or 1 is the same for any positive \( d \), so no estimates for the \( d_\Lambda \) follow from local consideration (near ends of integration interval for the \( f \)). Unlike the case for KPP model where \( d_\Lambda = 2 \) is pointed out by local analysis.

It does not seem feasible to use KPP-like profiles in FC because of the continuous spectrum of the velocities, thus long times of relaxing to steady state, and large widths with two exponential tails (thus no way to localize the “flame” compactly but still have the steep gradient region well resolved on the grid).

### 2.3 Step-function: velocities and widths

#### 2.3.1 Analytic solution

Analytic solution of (2.8) with constant diffusivity and step-function \( \Phi_0(f) \) (original implementation, Khokhlov (1995)) as found in Zhiglo (2007) is summarized below.

Translational invariance is fixed by considering a particular solution with \( f(\chi = 0) = f_0 \). In the region \( \chi > 0 \) \( \Phi_0(f) = 0 \) (no reaction) and solution is a diffusive exponential tail (analog of the preheating zone in standard Arrhenius flames) corrected
by matter expansion term in (2.8), only significant where \( f \) is not too small:

\[
f = 2\Lambda \left[ \left( 1 + \frac{2\Lambda}{f_0} \right) e^{d\chi} - 1 \right]^{-1} \approx \left( \frac{1}{2\Lambda} + \frac{1}{f_0} \right) e^{-d\chi}.
\] (2.22)

Last approximation is for \( \chi \gg \frac{1}{d} \ln (1 + 2\Lambda/f_0) \). When this region where \( f \) exponential decay is perturbed by expansion term is narrower than characteristic width of exponential decay \((1/d)\) flame width can be reasonably characterized by the slope of the profile \( f(\chi) \) at \( f = f_0 \); there the slope is maximal, thus this way one gets an estimate of the width from below:

\[
w_a = \frac{f_0}{|df/d\chi|_{f=f_0}} = \left[ d \left( 1 + \frac{f_0}{2\Lambda} \right) \right]^{-1}.
\] (2.23)

For comparison, to quantify how long the tail is compared to the rest of the flame, we also employ another width estimate,

\[
w_b = \frac{\chi(f = f_-) - \chi(f = 1)}{1 - f_-}
\] (2.24)

with \( f_- = 0.1 \). Analytical expression was found for \( w_b \); if \( f_0 \geq f_- \)

\[
w_b = \frac{1}{d} \left[ \ln \frac{1 + 2\Lambda/f_-}{1 + 2\Lambda/f_0} + d^2 \left( 1 + \frac{1}{2\Lambda} \right) \right].
\] (2.25)

This was computed using solution (2.22) at \( \chi > 0 \) and value

\[
\chi_1 = -d \left( 1 + \frac{1}{2\Lambda} \right)
\] (2.26)

for the rightmost point where \( f = 1 \), found directly from (2.8) integrated once over \( \chi \).

On \( \chi \in (\chi_1; 0) \) solution of (2.8) was found as

\[
f/\Lambda = -1 - \left( \frac{6\sigma}{d^2\Lambda} \right)^{1/3} \left( \frac{1}{3\sigma} + \frac{d}{d\sigma} \ln \left( I_{1/3}(\sigma) + BK_{1/3}(\sigma) \right) \right),
\] (2.27)

where

\[
\sigma = \left( \frac{2}{\Lambda} \right)^{1/2} \left( d\chi - \frac{d^2\Lambda}{2} \right)^{3/2}
\] (2.28)

and \( I, K \) are modified Bessel functions; \( B \) is an integration constant (real; another constant was fixed by requiring \( df/d\chi \) to be continuous at \( \chi = 0 \)).
This solution has to satisfy boundary conditions following from (2.5–2.6),

\[ f = \begin{cases} 
  f_0 & \text{at } \sigma_0 = \frac{d^2 \Lambda}{6} \\
  1 & \text{at } \sigma_1 = \left(1 + \frac{1}{\Lambda}\right)^3 \sigma_0 
\end{cases}, \quad (2.29) \]

thus leading to a transcendental equation defining sought for eigenvalue for \( d \) (entering through \( \sigma_0 \) and \( \sigma_1 \) arguments):

\[
\left( I_0 \left( 1 + \frac{f_0}{\Lambda} + \frac{1}{3\sigma_0} \right) + I_0' \right) \left( K_1 \left( 1 + \frac{1}{3\sigma_1} \right) + K_1' \right) \\
- \left( K_0 \left( 1 + \frac{f_0}{\Lambda} + \frac{1}{3\sigma_0} \right) + K_0' \right) \left( I_1 \left( 1 + \frac{1}{3\sigma_1} \right) + I_1' \right) = 0. \quad (2.30)
\]

Notation is \( I_0 = I_{1/3}(\sigma_0), K_1 = K_{1/3}(\sigma_1) \), etc. With definitions above this equation has a unique solution for \( d \) for every \( f_0, \Lambda \).

Figure 2.4: Flame velocities. The nine sequences \( d(\Lambda) \) correspond (top to bottom) to \( f_0 = 0.1, \ldots, 0.9 \) with step 0.1. The worst (\( f_0=0.1 \)) fit (2.36) is shown.

2.3.2 Results for velocities and widths

Numerical solutions of (2.30) are presented in Fig. 2.4. Figs. 2.5 and 2.6 show \( w_a \) and \( w_b \) for these two models. Flame profiles as in Fig. 2.1 were obtained by direct numerical integration of (2.10) with \( d \) from Fig. 2.4. Relative difference between \( d \)'s found numerically and analytically (i.e. by solving (2.30)) is less than \( 5 \times 10^{-3}\% \).
Figure 2.5: Flame width $w_a$ at the same $\Lambda$ and $f_0$. Larger widths correspond to larger $f_0$.

It was that large for $f_0 \geq 0.7$; for $f_0 \in [0.3; 0.6]$ the difference was of order $10^{-8}$, the accuracy required of the $d$ in numerical procedure (accuracy for solving (2.30) was set to $4 \times 10^{-16}$ and apparently these, “analytic” errors played no role), and monotonically increased to $20 \times 10^{-8}$ with $f_0$ further decreasing to 0.1. Errors in widths followed similar trends (and “numerical” widths were consistently larger than “analytical” ones, whereas velocities were smaller), though there was additional contribution from crude estimation (up to the whole grid) from integral curves $x(f)$ obtained from $p(f)$ via further trapezium integration; the discrepancy in $w_{a,b}$ was less than $8 \times 10^{-3}\%$.

For the SN Ia deflagration problem matter expansion is not large, thus it is worth trying to treat $1/\Lambda$ as a small parameter. A first-order correction to the solution $h_0 \equiv d(1/\Lambda = 0)^{-2}$ of (2.18) is (Zhiglo (2007))

$$d^{-2} = h = h_0 \left(1 + \frac{h_1}{2\Lambda} + O(\Lambda^{-2})\right), \quad h_1 = 5h_0 - e^{-1/h_0} \frac{2 + h_0 - h_0 f_0}{f_0 - e^{-1/h_0}}. \quad (2.31)$$

When $f_0$ is small as well this may be estimated with the aid of expansion from the end of Sec. 2.2.1 for $h_0$:  

$$h_1 = 5f_0 - e^{-1/f_0} \left(\frac{2}{f_0} + 1 - 6f_0\right) - e^{-2/f_0} \left(\frac{4}{f_0^2} + \frac{2}{f_0} - 6 - 6f_0\right) + O(e^{-3/f_0}/f_0^3), \quad (2.32)$$
Figure 2.6: Flame width \( w_b(f_0, \Lambda) = -\chi|_{f=0.1}^{1}/0.9 \). The order of \( f_0 \) (from larger to smaller \( w_b \) at \( 1/\Lambda = 20 \)) is 0.9, 0.1, 0.8, 0.7, 0.2, 0.6, 0.5, 0.3, 0.4.

this is usable up to \( f_0 \approx 0.3 \). Error of using (2.31) does not exceed 1% for \( 1/\Lambda \leq 1 \) (but \( d = h^{-1/2} \) must be used. Expanding \( d \) up to \( O(1/\Lambda) \) leads to far worse agreement.) At \( 1/\Lambda = 3 \) the error grows to 6.7% for \( f_0 = 0.3 \) (1.8% for \( f_0 = 0.2 \)); at \( \Lambda > 0.69 \) (SN Ia problem, \( \rho_{\text{fuel}} \geq 3 \times 10^7 \text{ g cm}^{-3} \)) it is within 2.1% for \( f_0 = 0.3 \), 0.16% for \( f_0 = 0.2 \). At these \( f_0 \) both expressions for \( h_1 \) give the same agreement.

2.4 Alternative flames with finite widths

In this section we present results for flame model (2.2) with non-constant diffusivity, \( K_0(f) = f^r \), \( r \in (0; 1) \), and step-function rate 2.11. It was studied in Zhiglo (2007) for a convenient in FC feature of flame profiles being localized, with no tails (as a further improvement over flame model due to Khokhlov (1995) studied in the previous section, which produces flames with “preheating” exponential tails, and KPP with long tails into both fuel and ash).

Like in Sec. 2.1 we are looking for a solution of eigenproblem (2.10) with \( p(0) = p(1) = 0 \) (as before \( p = -df/d\chi \equiv -\sqrt{K/R}df/dx \)). The above \( K_0(f) \) leads to \( f(\chi) \) \( C^1 \)-smoothly monotonically interpolating between \( f = 1 \) \( \forall \chi < \chi_1 = -d(1 + 1/2\Lambda) \) (fixing \( f(0) = f_0 \); \( f = 1 - (\chi - \chi_1)^2/2 + d(\chi - \chi_1)^3/2 + \ldots \) at \( \chi \to \chi_1^{+} \)) and \( f = 0 \) \( \forall \chi > \chi_2 \) \( (f = (rd(\chi_2 - \chi))^1/r(1 + O(\chi_2 - \chi)) \) at \( \chi \to \chi_2^{-} \).

\( \chi_2 \) and the total width \( w_c = \chi_2 - \chi_1 \) may be expressed in elementary functions of \( f_0, \Lambda \) and \( d \) for rational \( r \) (or as incomplete \( \Gamma \)–function in general). Values \( r = 1/2 \)
and \( r = 3/4 \) seem most adequate. Corresponding widths are

\[
\frac{w_{c,1/2}^1}{d} = \int_0^{f_0} f^{r-1} \left(1 + \frac{f}{2\Lambda}\right)^{-1} df \bigg|_{r=1/2} - \chi_1
\]

\[
= \frac{2}{d} \sqrt{2\Lambda} \arctan \left(\sqrt{f_0/2\Lambda} + d \left(1 + \frac{1}{2\Lambda}\right)\right),
\]

(2.33)

\[
w_{c,3/4}^3 = 2^{5/4} \Lambda^{3/4} d^{-1} \left[ \arctan \frac{(2f_0/\Lambda)^{1/4}}{1 - (f_0/2\Lambda)^{1/2}} + \ln \frac{(f_0/2\Lambda)^{1/2} - (2f_0/\Lambda)^{1/4} + 1}{(f_0/2\Lambda + 1)^{1/2}} \right]
\]

\[
+ d \left(1 + \frac{1}{2\Lambda}\right).
\]

(2.34)

In the last expression the branch of \( \arctan \) to be used is \( \arctan \in [0; \pi) \).

For any \( r \) in the limit \( \Lambda \to \infty \) (small expansion)

\[
w_{c,r} = \frac{f_0^r}{dr} \left(1 - \frac{f_0}{2\Lambda} \frac{r}{r+1} + \left(\frac{f_0}{2\Lambda}\right)^2 \frac{r}{r+2} + O\left(\frac{f_0}{2\Lambda}\right)^3\right) + d\left(1 + \frac{1}{2\Lambda}\right)
\]

\[
= \left(\frac{f_0^r}{rd_0} + d_0\right) + \frac{1}{2\Lambda} \left(d_0 \left(1 - \frac{h_1}{2}\right) - \frac{f_0^r}{rd_0} \left(\frac{f_0^r}{r+1} - \frac{h_1}{2}\right)\right) + O(\Lambda^{-2})
\]

(as in the \( r = 0 \) case \( d(f_0, r|\Lambda) = h^{-1/2} = d_0(1 + h_1 + \ldots)^{-1/2} \); \( d_0 = h_0^{-1/2} \), \( h_1 \), etc. are now some functions of \( f_0 \) and \( r \); as \( \Lambda \to 0 \) \( w_c \) diverges as

\[
w_{c,r} = \frac{(2\Lambda)^r}{d} \frac{\pi}{\sin \pi r} - \frac{f_0^r}{1 - r} \frac{2\Lambda}{d} + O(\Lambda^r) - \chi_1
\]

\[
= \frac{2^r \pi}{G_0 \sin \pi r} \Lambda^{-1}(1 - G_1 \Lambda) + \frac{G_0}{2} - \frac{2}{G_0} f_0^{r-1} + O(\Lambda)
\]

We used \( d = G_0 \Lambda (1 + G_1 \Lambda + o(\Lambda)) \) as in the step-function model with a standard diffusion term: \( d(\Lambda) \) dependence is qualitatively very similar. Fits of \( d(\Lambda) \) are presented in the next section.

For a range of \( \{f_0, r\} \) flame profiles deliver what they were expected to originally. Their width \( w_c \) may consistently serve as a measure of \( f \) gradients, and upon coupling (2.2) to the hydrodynamic equations one would really get reasonably uniform heat release within the flame width. On the contrary, for models with traditional diffusion term \( w_b \) was somewhat arbitrary quantity, most of it (for larger \( f_0 \) and KPP to a greater degree) might correspond to “tails” of a profile, and the heat release in FC would remain localized, contrary to the intention to more-or-less uniformly distribute it over a few cells near the modeled flame front. Some representative flame profiles are shown in Fig. 2.7; they are normalized to unit width (that is, reexpressed in terms
Figure 2.7: Normalized to unit width flame profiles with $f_0 = 0.6$ (left) and $f_0 = 0.2$ (right). The three curves for each $r$ correspond to $1/\Lambda \in \{0.16; 0.6; 3\}$, lower near $f = 0$ profiles for larger $1/\Lambda$.

of a new $X = (\chi - \chi_1)/(\chi_2 - \chi_1)$; resulting $\text{supp}(df/dX) = [0; 1])$. Three specific combinations $(f_0; r)$ are of particular interest for use in FC:

- $r = 1/2$. This has advantage that $f(x)$ behavior near $f = 0$ is the same as near $f = 1$, thus we are unlikely to introduce new problems (compared to the original $r = 0$ scheme). $f_0 = 0.2$ is then convenient as the $f(x)$ shape is least sensitive to $\Lambda$ in its range of immediate interest, $1/\Lambda \in [0; 2]$.

- $r = 3/4, f_0 = 0.6$. For the $\Lambda$’s of interest corresponding flame profiles seem most symmetric overall with respect to $f \mapsto 1 - f$; this is perhaps a better realization of the above idea: as the whole $w_c$ width is to be modeled on a few integration cells this approximate global symmetry seems more adequate to consider than the symmetry of minute regions near $f = 0$ and $f = 1$.

- $r = 3/4, f_0 = 0.2$. Profile gradients are still uniform enough on $[0.1; 0.9]$, they drop to zero in a regular manner within reasonable $\Delta \chi \leq 0.25 w_c$. At $f_0 = 0.2$ the profiles seem least sensitive to $\Lambda$, ensuring consistent performance in all regions of the star.

As another possibility it might seem more physical to write the reaction-diffusion equation as

$$\frac{\partial (\rho f)}{\partial t} + \nabla (\rho f u) = \nabla \left[ \rho \tilde{K} K_0(f) \nabla f \right] + \rho R \Phi_0(f),$$

with density appearing under divergence in the third term, $\nabla (\rho K \nabla f)$. This case was studied as well. Normalized to unit total width flame profiles are more sensitive to $\Lambda$ than the ones corresponding to (1.3); such a model is also less tractable analytically. The model with diffusion term of this form and with $K(f) = const$ was also studied as a possible alternative to the original one (2.2). Asymptotic behavior of $d$ and
the widths at small and large $\Lambda$ are the same as presented in the previous section, hence the decision to stick to the original (apparently consistently performing) model. Physical transport coefficients change after flame passing, making it questionable if putting the $\rho$ under $\nabla$ really makes the model in this paragraph “more physical”, in view of the artificial $K_0(f)$ dependence chosen vs effective $K(f)$ for turbulent burning (the latter are higher in the ash, qualitatively similar to our $K_0(f)$.)

2.5 Suggestions for implementation

2.5.1 Fits of the flame speed dependence on expansion

Analytically found asymptotes for $d(\Lambda)$ (Sec. 2.3.2) at small $1/\Lambda$ do not provide enough accuracy to be used for flame tracking in outer layers of WD (although the errors are within 1% for $f_0 = 0.2$ and $1/\Lambda < 2$.) Next order in $1/\Lambda$ seems sufficient at $f_0 \leq 0.2$ yet computations become too involved in $r \neq 0$ case (Sec. 2.4). More importantly, flame capturing as presented is a general method, thus it is desirable to get results with larger range of validity in a ready to use form. In this section we present fits neatly interpolating between small and large $\Lambda$ regions and then summarize the procedure for getting $R$ and $\tilde{K}$ for (1.3) in the SN Ia simulations.

$$d(\Lambda) = \frac{m_1}{1 + m_2/\Lambda} + \frac{m_3}{(1 + m_4/\Lambda)^2}$$ (2.36)

with $m_{1,4}$ obtained at each $f_0$ to minimize the mean square deviation (with weights proportional to actual $d(\Lambda)$) was the simplest fit found. The values shown in the graph below guarantee 0.2% accuracy for each $f_0 \in \{0.01; 0.025(0.025)0.975\}$ and $\Lambda \in [10^{-3}; 10^5]$ studied (for any $\Lambda$ in fact, as comparison of asymptotes shows). For $f_0 > 0.3$ agreement is significantly better. I have not succeeded to find a simple expression for $m_{1,4}(f_0)$ providing good agreement for all expansions; this is due to delicate interplay between the two terms near $1/\Lambda = 0$. Complicated form of $m_{1,4}(f_0)$ is related to different significance of the two asymptotic regions in the fit: for $f_0 = 0.01$ the $d(\Lambda)$ becomes reasonably linear ($d/\Lambda \approx \text{const}$) only at $1/\Lambda > 300$, whereas for $f_0 > 0.5$ this happens at $1/\Lambda \geq 2$. To overcome this a number of other possible fits were tested. In short, 3-parameter fits were significantly less accurate (though 3% accuracy was achieved, uniformly on $\Lambda \in (0; \infty)$), fits with more than 4 parameters did not yield significant improvements; none of accurate fits considered admitted simple expressions for its coefficients in terms of $f_0$.

This is not a major issue as $f_0$ is a parameter one can fix at some convenient value throughout the simulation. $f_0 = 0.2$ seems most suitable for the finite width flames with $r = 1/2$ or $3/4$, as discussed in Sec. 2.4. For constant diffusivity and step-function burning rate of Khokhlov (1995), with new coefficients prescription described here, we suggest using $f_0 = 0.2$, based on the following consideration.
Figure 2.8: Fit (2.36) parameters for $r = 0$ (the first 4 curves according to the legend) and $r = 3/4$ (next 4). $M_{1,3} = m_{1,3}\sqrt{f_0}$.

In Khokhlov (1995) $f_0$ was fixed at 0.3, which essentially yielded thinnest flames throughout the $\Lambda$ range in the problem (A. Khokhlov, private communication. Note that this agrees with our findings, cf. Fig. 2.6.) The width of the “flame” of the original model is $W \approx w_b(f_0, \Lambda) \beta \Delta x$; $\beta = 1.5$ was used, $\Delta x$ is a grid size; it changes with expansion $\Lambda$ proportionally to $w_b(f_0, \Lambda)$, the magnitude of this change may be seen in Fig. 2.6. Now, the prescription I advocate normalizes width as well as the flame speed\(^3\), thus the logical criterion for $f_0$ to suggest would be the fastest tail (near $f = 0$) decay in the profile normalized to unit width $w_b$, for the case of traditional FC realization. This translates to smallest $1/w_b \rho$. This, however, can be made arbitrarily small by taking sufficiently small $f_0$; we suggest to stick to $f_0 = 0.2$, as this yields $1/w_b \rho$ least sensitive to $\Lambda$ in $(0.4; \infty)$; flame profiles normalized to unit $w_b$ also exhibit fairly low sensitivity to $\Lambda$. At smaller $f_0$ at small $\Lambda$ ($\leq 0.5$) profile shapes on $f \in [0.1; 1]$ become rather nonlinear, making the choice of $w_b$ as a measure for “width” more questionable.

\(^3\) We can now also easily quantify the error in flame speed achieved in Khokhlov (1995): the values of $K$ and $R$ used there result in actual flame speed larger than the prescribed one by a factor of $d(f_0, \Lambda)\sqrt{f_0}$. It is reasonably close to 1 at small $1/\Lambda$ and $f_0 = 0.3$: the flame speed that original model produces is 7\% smaller in the WD center. However it is $\sim 1.45$ times smaller when $\rho = 3 \times 10^7$, at 0.5C+0.5O composition.
Flame speed when matter expansion may be neglected, a solution of (2.18), value of which appears in expansion (2.31) for \( d \) at small \( \Lambda \), can be approximated as

\[
d_0 = \left[ \frac{1 - f_0^{1.4448} \exp(0.58058(1 - f_0^{-1}))}{f_0} \right]^{0.5},
\]

with errors of \( \leq 0.64\% \) for any \( f_0 \). For \( r = 1/2 \) and \( r = 3/4 \)

\[
d_0 = \left[ 2 (1 - f_0) f_0^{-1} \right]^{1/2}
\]

provides 1.5% accurate fits.

| \( f_0 \) | \( r \) | \( m_1 \) | \( m_2 \) | \( m_3 \) | \( m_4 \) | \( \epsilon_d, 10^{-4}\% \) |
|---|---|---|---|---|---|---|
| 0.1 | 2.9248 | 0.081016 | 0.23690 | 0.32153 | 90 |
| 0.2 | 1.9588 | 0.14574 | 0.26929 | 0.42824 | 66 |
| 0.3 | 1.4620 | 0.19389 | 0.32605 | 0.39759 | 11 |
| 0.4 | 1.1889 | 0.24193 | 0.30495 | 0.39044 | 6.1 |
| 0.5 | 1.0312 | 0.29358 | 0.23117 | 0.40545 | 11 |
| 0.6 | 0.90646 | 0.34328 | 0.15479 | 0.42613 | 7.2 |
| 0.9 | 0.44817 | 0.46634 | 0.015034 | 0.48381 | 5.3 |
| 0.2 | 3/4 | 1.1683 | 0.14139 | 0.40205 | 0.37378 | 56 |
| 0.6 | 3/4 | 0.81846 | 0.34834 | 0.14334 | 0.42779 | 9.0 |
| 0.2 | 1/2 | 1.3969 | 0.14439 | 0.35064 | 0.39886 | 52 |

Table 2.1: Parameters of fit (2.36) for \( d(\Lambda) \) for flame models with burning rate (2.11) and constant \( K \) (\( r = 0 \) effectively, as in the original FC model: first 7 entries) and \( K = f^r \) (last 3 lines). The last column shows the maximum relative discrepancy between the \( d(\Lambda) \) and its fit (with \( m_1...4 \) truncated exactly as in the Table) at \( \Lambda \in [1/3; 20] \), \( \epsilon_d = (|\Delta d|/d)_{\text{max}} \).

The fit parameters \( m_1...4 \) for \( f_0 = 0.1...0.9 \), as well as for the \( \{f_0, r\} \) values suggested in Sec. 2.4 optimized for \( \Lambda \in [1/3; 50] \) are summarized in Tab. 2.1.

### 2.5.2 Prescribing normalizations of diffusivity and reaction rate for propagating the “flame”

The strategy for using the results of this chapter in FC is as follows. One picks the favorite flame model; this means a pair \( \{f_0, r\} \) for the models considered in this chapter (based on step-function burning rate, Eq. 2.11, and diffusivity \( K = f^r \)). One finds corresponding dimensionless steady flame speed \( d \) and width \( w \), in each computational cell. For models studied in this chapter, this is accomplished by taking
From Table 2.1 corresponding to the \( \{ f_0, r \} \) used, (2.36) then defines \( d \) based on local \( \Lambda \) (2.4), and (2.25) (or (2.33) for \( r = 1/2 \), or (2.34) for \( r = 3/4 \)) determines dimensionless width \( w \) (\( w_b \) or \( w_c \)). Next, one defines needed \( D_f(\Delta) \) (based on local density, gravity, etc; e.g. (1.1), \( \Delta \) meaning the grid spacing).

\[
\dot{K} = \frac{D_f}{d} \frac{W}{w}, \quad R = \frac{D_f}{d} / \frac{W}{w},
\]

(2.37)

(where \( W \) is a desired flame width, say \( 4\Delta \)) will then yield scale-factors for the parameters (2.7) appearing in the equation governing \( f \) evolution, (1.3). This equation with so defined coefficients when coupled with standard equations of hydrodynamics will lead to a “flame” with the desired speed \( D_f \) and width \( W \) within the approximations adopted in this chapter (steady 1D burning, pressure and \( H\rho \) approximately constant across the flame, discretization effects neglected).

2.6 Nonstationary numerical tests

Here we briefly present numerical verification of the key results of the previous sections, which were based on steady-state consideration. The goal is to see how well the prescribed velocity and width were achieved when prescriptions of Sec. 2.5 were used. Flame profile sensitivity to the expansion parameter is also studied here in realistic non-steady simulations.

2.6.1 Flame speed and width

For the simulations presented below ALLA code developed by A. Khokhlov [Khokhlov (1998, 2000)] was used. The simulations were performed in 1D without gravity, with actual WD equation of state, and heat release corresponding to complete \( 0.5C+0.5O \) burning to the NSE composition at a given density. The 1D integration domain (called “tube” below) was closed at one end (reflecting boundary conditions); 4 cells of hot ash were placed at this end for ignition, in hydrostatic equilibrium with cold fuel in the rest of the tube. At the other end outflow conditions were imposed.

Four models were studied: the three proposed at the end of Sec. 2.4, and a model with constant diffusivity and \( f_0 = 0.2 \). For each model the simulation was run for 4 densities, \( \rho = \{ 3 \times 10^7; 10^8; 3 \times 10^8; 2 \times 10^9 \} \) g cm\(^{-3} \). These yielded expansions \( 1/\Lambda = \{ 1.442; 0.7322; 0.3975; 0.1669 \} \) respectively (released heat was \( q = \{ 7.399; 5.736; 4.469; 3.382 \} \times 10^{17} \) ergs g\(^{-1} \)). The coefficients in Eq. (2.2) were determined from Eq. (2.37) with \( D_f \) set constant 80 km s\(^{-1} \) for all runs, \( W = 4 \) cells. \( d \) was defined using (2.36) with relevant coefficients from Table 2.1, exact expressions for \( w_b \) (for Model \( \{ f_0, r \} = \{ 0.2, 0 \} \)) or total width \( w_c \) (for the three finite width models emphasized in Sec. 2.4) were used as \( w \) in Eq. (2.37).
Table 2.2 summarizes the results. \( D \) is the measured flame speed, determined as \( D = \frac{1}{\rho_{\text{fuel}}} \frac{d\rho_{\text{ash}}}{dt} \), \( W_{1,2,3} \) characterize the flame width. These widths were determined in the following way (following A. Khokhlov): at each timestep from 2001 to 10000 a number of cells with \( f \) between \( f_d \) and \( f_u \) was found, and then averaged over these 8000 steps. \( W_1 \) was obtained this way while choosing \((f_d; f_u) = (0.1; 0.9)\), \( W_2 \) with \((f_d; f_u) = (0.01; 0.99)\), and \( W_3 \) with \((f_d; f_u) = (0.001; 0.999)\). Steady state profile had been established by timestep 500; at timestep 10000 the flame was still far enough from the open tube end. For all the results in this Table the tube length was 620 km, corresponding to 256 integration cells. The last timestep (10,000) corresponded to 1.8–2.6 s depending on density.

| \( \rho \)     | \( D \) (in km s\(^{-1}\)) | \( W_1 \) (in cells) | \( W_2 \) (in cells) | \( W_3 \) (in cells) | \( D \) (in km s\(^{-1}\)) | \( W_1 \) (in cells) | \( W_2 \) (in cells) | \( W_3 \) (in cells) |
|----------------|-----------------------------|----------------------|----------------------|----------------------|-----------------------------|----------------------|----------------------|----------------------|
| \( 3 \times 10^7 \) | 76.4                        | 2.69                 | 3.97                 | 4.96                 | 73.2                        | 2.56                 | 3.92                 | 5.20                 |
| \( 1 \times 10^8 \) | 77.8                        | 2.70                 | 4.02                 | 4.92                 | 74.2                        | 2.59                 | 3.99                 | 5.24                 |
| \( 3 \times 10^8 \) | 78.5                        | 2.67                 | 4.04                 | 4.88                 | 75.0                        | 2.61                 | 4.01                 | 5.22                 |
| \( 2 \times 10^9 \) | 78.9                        | 2.64                 | 4.04                 | 4.70                 | 75.6                        | 2.61                 | 4.01                 | 5.12                 |

\( (r; f_0) = (0.75; 0.2) \)

| \( (r; f_0) = (0.5; 0.2) \) | \( (r; f_0) = (0; 0.2) \) |
|-----------------------------|-----------------------------|
| \( 3 \times 10^7 \)       | 76.4                        | 2.55                 | 3.77                 | 4.75                 | 76.7                        | 3.18                 | 5.00                 | 6.42                 |
| \( 1 \times 10^8 \)       | 78.2                        | 2.58                 | 3.85                 | 4.76                 | 78.2                        | 3.22                 | 5.23                 | 6.81                 |
| \( 3 \times 10^8 \)       | 78.9                        | 2.57                 | 3.88                 | 4.75                 | 78.9                        | 3.23                 | 5.38                 | 7.07                 |
| \( 2 \times 10^9 \)       | 79.4                        | 2.54                 | 3.91                 | 4.61                 | 79.4                        | 3.22                 | 5.49                 | 7.30                 |

Table 2.2: Flame velocities, \( D \) (in km s\(^{-1}\)), and widths \( W_{1,2,3} \) (in cells) at different densities \( \rho \) (in g cm\(^{-3}\)) for 4 flame models

To see if statistics was sufficient the same simulation was run with 16 times longer tube (divided into 4096 cells) for 160000 timesteps for two of the models. Flame speed and the three widths agreed within 0.1% (these were averaged over last 158000 steps in these long runs) with those in Table 2.2. Therefore larger than 4 cells \( W_3 \) for the 3 finite-width models (as well as \( D \) distinct from 80 km s\(^{-1}\)) must be attributed to discretization: as \( f \) changes from 0 to 1 mostly within 4 cells one generally would expect errors in estimating gradients via finite differences to affect the flame profile and propagation speed. To quantify this discretization effect the model with \( r = 0.75, f_0 = 0.2, \rho = 3 \times 10^7 \) g cm\(^{-3}\) was run in 1D domains 512, 1024 and 2048 cells long, with \( D = 80 \) km s\(^{-1}\) and \( W \) equal to 8, 16 and 32 cells respectively (these \( D \) and \( W \), as always, define \( \tilde{K} \) and \( R \) via (2.37), and are the values for flame speed and width one hopes to get with the simulated flame). The results are summarized in Table 2.3. These (together with the first quartet in Table 2.2) illustrate the trend. In part, for the flame width of order 16 cells or wider the \( W_3 \) becomes smaller than the prescribed \textit{total} flame width, as it should; the difference
between the prescribed flame speed $D$ and the actual value also tends to zero when
the number of zones in the flame increases. The same holds for different densities: say,
measured flame speed for the same ($r = 0.75, f_0 = 0.2$) model at $\rho = 2 \times 10^9 \text{g cm}^{-3}$
is $\{78.8; 79.4; 79.9\}$ km s$^{-1}$ for $W = \{8; 16; 32\} \Delta$ respectively.

| $W$ | $D$ | $W_1$ | $W_2$ | $W_3$ |
|-----|-----|-------|-------|-------|
| 8   | 77.3| 5.25  | 7.48  | 8.40  |
| 16  | 79.1| 10.57 | 14.67 | 15.87 |
| 32  | 80.0| 21.32 | 29.27 | 31.53 |

Table 2.3: Flame velocities and widths at different prescribed flame widths $W = x|_{f=1}^{0+}$ (in cell sizes, $\Delta$). ($r; f_0$) = (0.75; 0.2), $\rho = 3 \times 10^7 \text{g cm}^{-3}$.

This study shows that really the difference between the prescribed flame speed
and the actual one achieved in simulations is due to a small number of cells within
the flame. The discrepancy can be corrected for by tuning the $d$ and $w$ values in
(2.37), that is adjusting our analytic prescription for the coefficients in (1.3) or (2.2)
with additional ($\Lambda$-dependent) factors. This will be done in the next Chapter for
flame models studied there.

### 2.6.2 Flame profiles

Two of the models in Sec. 2.4 were proposed for use for the low sensitivity of their
flame profiles to the expansion parameter. Fig. 2.9 shows that this nice property
is not spoiled by the discretization effects, and further clarifies the nature of longer
profile tails in discretized setting. For each model, $f_0 = 0.2$, and $r = 0.75$ or 0.5, the
values of $f$ were recorded near the flame position for 4 different timesteps; for each
timestep the set of values $f(x_i)$ was first renormalized in $x$ direction by dividing all the
$x_i$ by $4\Delta$, thus normalizing the numerical profiles to unit total width (more precisely,
they would have had unit width if there had not been discretization corrections); then these renormalized profiles were translated in $x$ direction so that they least
deviated from the steady-state profiles (Fig. 2.7). This procedure was performed
with the 2 models displayed in Table 2.2, for the same 4 densities. As Fig. 2.9
shows the numerical profiles with 4 cells wide flames (1) closely follow corresponding
steady-state (continuous) profile at all times (apart from the longer tail), and (2)
as a consequence, are insensitive to density. These numerical profiles, further, show
about the same density independence for the two models, $(r,f_0) = (0.5,0.2)$ and
$(0.75,0.2)$, which suggests to stick to the former one because of its more symmetric
profile.

We conclude that all results of this chapter agree for different methods used for
their derivation: analytical versus numerical solution of steady-state (continuous)
Figure 2.9: Theoretical (steady-state; black curve) and numerical flame profiles (red dots) normalized to unit theoretical width. Numerical profiles are represented by values $f(x_i)$ near the flame position for 4 timesteps at 4 densities. For the $(r; f_0) = (0.75; 0.2)$ model the dots are differentiated according to fuel density: circles correspond to profiles at $\rho = 2 \times 10^9$ g cm$^{-3}$, hexagons to $3 \times 10^8$, stars to $1 \times 10^8$, and triangles to $3 \times 10^7$.

problem versus direct numerical simulation using full hydro-solver ALLA. All discrepancies observed are clearly related to their respective causes: errors of numerical integration of ODE’s in steady-state approach (effects of which shown to vanish with refining resolution; these errors are within $10^{-2}\%$ for flame velocities and widths when bulk integration step is $\Delta f = 10^{-5}$, further refined up to $\Delta f_{\text{ref}} = 10^{-8}$ near peculiar points of defining ODE (2.10) — the setup we used for most calculations); discretization effects in direct numerical estimates in non-steady setup. Corrections due to discretization were seen to be negligible when the “flame” is resolved on 16 or more cells, but they were up to 10% in observed flame speed for some flame models when prescribed total flame with $W$ was set to 4 cells, and more than that in flame widths. The effect of discreteness of non-steady simulation on flame width was seen to be mostly due to longer tails in flame profiles (due to numerical diffusion). These cross-checks between different approaches provide trustworthy estimates for accuracy of corresponding methods, what resolution for numerical integration of eigenvalue problem is sufficient, what are discretization corrections for models with different flame profiles. The same checks are performed in the following chapters for 2 new flame models, for which the methods described in this chapter are used for similar calibration, needed for use in FC and for head-to-head comparisons of numerical and physical non-steady effects between the models (for which parameters like $D$ and $W$ are fixed the same for all comparisons performed). We study numerical
noises the flame models introduce in 1D simulations in Chap. 3, isotropy of flame propagation and flame surface instabilities in 2D and 3D in Chap. 4.
CHAPTER 3
FLAMES IN NON-STEADY SIMULATIONS:
NUMERICAL NOISES IN 1D

This chapter and the next one are devoted to studying features of model flames in non-steady simulations. Non-steady properties we observe (and describe below) are visibly separated into physical (thus expected) effects, and effects related to numerics. The latter are numerical noises, like sound waves generated and flame speed fluctuating in time, with periods directly related to flame propagation with respect to the grid; anisotropic flame propagation in 2D/3D setting, with grid dictated special directions. The numerical artifacts are clearly undesirable, they disturb and systematically deviate numerical model behavior from physically sound one, having nothing in common with reality. Finding numerical realization showing least possible amount of these numerical artifacts is necessary, and is one of important goals of our study.

Other effects we observe also deviate artificial flame behavior in simulations from what would seem ideal for flame capturing applications; effects of this class, however, are expectable physical phenomena for any diffusion-reaction flames. These effects include dependence of flame propagation speed upon local flame curvature (Markstein effect, Markstein (1964)); growth of wrinkles on initially smooth flame surface, hydrodynamic instability of the type (LD for short) studied in Landau (1944); Darrieus (1938). These effects depend to a degree on the model diffusivity and reaction rate functions; no model, however, is free of these effects. Real physical flame is also an example of reaction-diffusion system, albeit more complicated; its propagation shows the same physical effects. Ideal flame capturing scheme therefore would be not the one showing no effects of this physical class, but the one demonstrating these effects with magnitude equal to that of (smeared over grid cell scale) physical flame region. Results below, Chap. 4, demonstrate that features of LD instability depend strongly on the parameters of the model; we cannot hope that some random flame model physical features will match quantitatively those of real physical flame region. Detailed study of real flame is required to find its Markstein length, critical length and growth rate with respect to hydrodynamic instability; only then one would be prepared to analyze deviations from corresponding features of artificial flame model (studied in this work), and try to correct for these deviations.

Some instabilities, like Rayleigh-Taylor, depend on density contrast across the flame zone, and do not depend significantly on specifics of density distribution in the transient (flame) region, as long as corresponding instability scale exceeds this transient region width. This is not the case for a thick “flame” used in FC, yet it is the task of subgrid model to prescribe renormalized effective “turbulent flame speed” to correct for this intricate subgrid geometry being smeared out by the thick artificial “flame”. This is not related to the scope of the thesis, this subgrid pre-
cription should be the same for any flame model; it may only slightly depend on specifics of density distribution within the “flame”, which distinguishes one model from another (assuming the same widths of the flames they produce). Response of the flame to front curvature (Markstein effect) and LD instability, on the other hand, do depend significantly on specific flame model. They also depend strongly on the flame width, thus are expected to be different for the model thickened “flame” and for the real thin nuclear (or chemical) flame. What is average manifestation of these real hydrodynamic effects on large, resolved scales, whether it is may be comparable to corresponding effects observed for thickened flame with the width of order of characteristic width of the convoluted with instabilities physical flame brush — is an interesting topic to study, however this is not touched upon in the thesis.

With qualitative understanding above in mind, we study several flame models in real non-steady simulations without gravity (to have constant fuel density throughout the simulation, and to avoid complicating the observations with RT instability, which is essentially the same for different flame models). This chapter deals with numerical noises which are 1D in nature. No physical 1D instabilities are known for flame models of the type we consider (with only one significant transfer coefficient); we did not observe any in simulations performed.

We describe and calibrate (using methods of Chap. 2) two new flame models in Sec. 3.1. We present results for sound waves produced by these models, as well as by the model studied in Chap. 2 (based on step-function burning rate (2.11), and power-law diffusivity $K_0(f) = f^r$, $r = 3/4$) in 1D simulations in Section 3.2, after describing numerical methods used. A feature is identified in the burning rate (namely discontinuity), which causes noise in simulations; this noises are too intensive for the model used in Khokhlov (1995) as well as in other models studied in Chap. 2, based on step-function burning rate. The 2 new models introduced in Sec. 3.1 produce acceptable level of noise; this was a criterion for selecting them for further study in the next chapters, where 2D and 3D behavior is analyzed.

3.1 Models studied: definition and steady state parameters

3.1.1 Definition of the models

As discussed in Chap. 2 certain features of artificial flame system are desirable for flame capturing applications. In part, we want the system to have a unique eigenvalue for $D_f$, and want flame profiles to have finite width (without exponential or power-law tails), with reasonably constant $df/dx$ within the “flame”. This limits possible $K(f)$ and $\Phi(f)$ in (1.3) suitable for flame capturing.

As a brief overview, two realizations of (1.3) were used in literature before Zhiglo (2007). Diffusivity is constant in both, $K(f) = \bar{K} = \text{const}$, the realizations differ by reaction rate forms. The model originally proposed in Khokhlov (1995) has step-
function \( \Phi(f) \), (2.11). This yields “flame” having an exponential tail into fuel (this tail, where \( f < f_0 \), represents “preheating zone”); \( D_f \) eigenvalue is unique and exists for all \( \tilde{K}, R, f_0 \). Another flame model tried in astrophysical literature (Dursi et al. (2003)), based on KPP burning rate [Kolmogorov et al. (1937)] \( \Phi(f) = Rf(1 - f) \), has continuous \( D_f \) spectrum (for any \( D_f > 2\sqrt{\tilde{K}R} \) there exist a solution of (2.3) satisfying physical boundary conditions), and two infinite tails in eigenfunctions \( f(x) \): \( f \) approaches 0 and 1 exponentially as \( x \) goes to \( +\infty \) or \( -\infty \) respectively.

In Sec. 2.4 we proposed a new flame model based on the original step-function burning rate, but with diffusivity dependent on \( f \):

\[
\Phi(f) = R\Phi_0(f) = \begin{cases} 
R & \text{for } f_0 < f < 1 \\
0 & \text{for } f < f_0
\end{cases}; \quad K(f) = \tilde{K}f^r. \tag{3.1}
\]

This diffusion-reaction model has a unique steady-state speed \( D_f \), like the original one (Khokhlov (1995); effectively a limit case of (3.1) with \( r = 0 \)), and for \( r > 0 \) corresponding flame profile is finite: the region, “flame”, where \( f \) is neither 0 nor 1 has finite width. We proposed to use this model with

\[
f_0 = 0.2, \quad r = 0.75, \tag{3.2}
\]

as these parameters led to flame profiles having the same shape for any \( \Lambda \in [0.25; \infty) \). This encompasses all physically interesting range of fuel densities for deflagration in a WD, from central density of \( \sim 2.2 \times 10^9 \text{g cm}^{-3} (\Lambda \approx 6.2) \) down to \( \sim 3 \times 10^6 \text{g cm}^{-3} \) (considering half-carbon, half-oxygen composition). We will present results for this \((f_0, r)\) pair only, as this type of model turns out to be quite noisy for any \((f_0, r)\) (including original model in Khokhlov (1995), corresponding to pair \((f_0, r) = (0.3, 0)\)), significantly worse than the other two models we will study (and thus of limited interest for use in flame tracking). We refer to this model as Model A in the following.

The second model we analyze in this paper is based on a modification of KPP burning rate with constant diffusivity,

\[
\Phi(f) = R(f - \epsilon_f)(1 - f + \epsilon_a) (0 < \epsilon_f, \epsilon_a < 1), \\
K(f) = \tilde{K} = \text{const}, \tag{3.3}
\]

dubbed “shifted KPP” (sKPP for short) at FLASH center meetings where it was invented, due to the nature of corrections to KPP burning rate, significant only when \( f \) is close to either 0 or 1; these corrections effectively cut exponential tails of original, “not shifted” KPP-flame profile (corresponding to \( \epsilon_f = \epsilon_a = 0 \)) rendering flame localized in space, like model (3.1). Besides, this model has unique flame
propagation speed, another advantage over original KPP model\footnote{These properties, as well as asymptotic behavior of the flame profile of this model (namely, \( f(x) \) is parabolic near both flame boundaries, \( f = 0 \) and \( 1 \)), may be found in qualitative analysis in Sec. 2.2.3.}. We will describe the results for this model for \( \epsilon_f = \epsilon_a \) case: these 2 parameters have similar effect on model characteristics due to the symmetry of its burning rate \( \Phi(f) \), and there was found no significant advantage when using different values in the pair, \( \epsilon_f \neq \epsilon_a \). \( \epsilon_f = \epsilon_a = 10^{-3} \) produces optimal results in terms of 2D/3D behavior and 1D noises (see below).

The third model studied, Model B, the one we recommend for use in flame capturing based on its behavior in multidimensional simulations, is specified by

\[
\begin{align*}
\Phi(f) &= R_f s_f (1 - f)^{s_a} (f - c(\Lambda)) \\
K(f) &= \bar{K} f^r_f (1 - f)^{r_a},
\end{align*}
\]  

(3.4)

(3.5)

with

\[
\begin{align*}
s_f &= 1, s_a = 0.8, r_f = 1.2, r_a = 0.8,
\end{align*}
\]  

(3.6)

and \( c(\Lambda) \in [0.005, 0.3] \) determined locally as a function of expansion parameter for fuel/ash at given local pressure and fuel composition. This model has a unique steady-state flame propagation speed (when \( c(\Lambda) > 0 \)); flame profiles are localized, and do not have long tails (in contrast with model (3.3)); they look similar to profiles of model (3.1–3.2). Term \( c(\Lambda) \) was selected to minimize flame propagation anisotropy and hydrodynamic flame surface instabilities in 2D at different fuel densities (Chap. 4). Reasonable results were achieved with \( c(\Lambda) \) defined as a spline:

\[
\begin{align*}
c &= 0.005 \text{ for } 1/\Lambda < 0.515 \\
c &= 0.3 \text{ for } 0.81 < 1/\Lambda < 1.5 \\
c &= 0.2 \text{ for } 1/\Lambda > 1.9,
\end{align*}
\]  

(3.7)

(3.8)

(3.9)

and continuously linearly changing between these \( \Lambda \) intervals (see Appendix for explicit formulae). Exponentials (3.6) were chosen based on steady-state considerations and non-steady properties. \( s_f, s_a \gtrsim 0.7 \) for \( \Phi(f) \) to go to 0 fast enough at \( f \to 0 \) and 1 (to avoid significant 1D noises, see Sec. 3.2). \( s_a < 1 \) for the model to have a unique eigenvalue for flame speed. \( r_f > 1 \) for the flame not to have infinite tail into fuel. Somewhat larger \( r_f \), up to 2, produce acceptable results as well, yet no improvement can be obtained in 2D behavior. \( r_a = 0.8 \) was chosen for reasonably symmetric flame profile, with nearly constant \( df/dx \) within. Flame profiles for this model (Model B), and Model sKPP (3.3) are shown in Fig. 3.4 below.
3.1.2 Steady-state and numerical calibration of the models: method

To use flame model in simulations for flame tracking one has to know how to prescribe model parameters in such a way so that the model flame propagated with required velocity, and had prescribed width. For this calibration we use the same approach as in Chap. 2: by factoring burning rate and diffusivity into constant dimensionful scale-factors and (\(f\)-dependent in general) dimensionless form-factors (Eq. 2.7),

\[
\Phi(f) = R\Phi_0(f), \quad K(f) = \tilde{K}K_0(f)
\]

we get an eigenproblem (Eqs. (2.8), (2.5), (2.6)) for finding dimensionless flame speed

\[
d = \frac{D_f}{\sqrt{\tilde{K}R}}
\]

and flame profile \(f(\chi)\) in terms of dimensionless coordinate \(\chi = \frac{x}{\sqrt{r/\tilde{K}}}\) along flame propagation. This problem is solved by numerical integration of the ODE and using Newton-Raphson method for obtaining the eigenvalue of \(d\), for which boundary conditions are satisfied. The procedure and resolutions used are the same as discussed in Chap. 2.1.2.

To quantify the profile shape, whether the slope of \(f\) within the flame profile is approximately constant, or if the profile has long tails, with regions of large and small gradients of \(f\) having comparable spatial scales, we calculate widths defined in 3 different ways:

\[
\begin{align*}
    &w_1 = \chi|_{f=0.9}^{0.1} = \chi(f=0.1) - \chi(f=0.9) \\
    &w_2 = \chi|_{f=0.99}^{0.01} \\
    &w_3 = \chi|_{f=0.999}^{0.001}
\end{align*}
\]

Having found \(d\) and \(w\) (in any convenient sense, e.g. any of \(w_{1,2,3}\)) one has a simple way to normalize the flame model to yield prescribed flame speed \(D\) and width \(W\) (same definition of “width” must be used for physical width \(W\) for simulations, and dimensionless width \(w\); say, both between \(f = 0.1\) and \(f = 0.9\)). Namely (see Sec. 2.5.2), one must use (1.3) for flame tracking, with burning rate and diffusivity (2.7), where scale factors are determined through Eq. 2.37:

\[
\tilde{K} = \frac{D_f}{d} \frac{W}{w}, \quad R = \frac{D_f}{d} \left/ \frac{W}{w} \right.
\]

(3.11)

To summarize, for any flame model (\textit{i.e.} selected for use dimensionless \(\Phi_0(f)\) and \(K_0(f)\)) one finds corresponding \(d\) and \(w\), and then, using (2.37), finds normalization factors for burning rate and diffusivity, \(R\) and \(\tilde{K}\), which lead to prescribed “flame” (1.3) speed and width.

Same parameters \(d\) and \(w\), defining proper normalization of \(K(f)\) and \(\Phi(f)\), may be found directly numerically, by simulating flame propagation in 1D, finding \(\tilde{K}\) and \(R\) correctly yielding some chosen \(D\) and \(W\), and then reversing (3.11) to find \(d\) and
$w$; these latter can be used later on for getting $\tilde{K}$ and $R$ yielding any physically motivated flame speed. Such numerically found $d$ and $w$ differ slightly from exact $d$ and $w$ obtained by solving eigenvalue problem: the former, numerically found $d$, is essentially the eigenvalue of discretized system (2.8), where spatial derivatives of $f$ are represented by finite differences on a grid, with total flame width of just $\sim 4$ grid spacings. Flame profile of discretized problem also deviates from continuous one, exact eigenfunction of steady-state boundary value problem. Most notably, one gets longer tails near $f = 0$ and $f = 1$, thus $w_{1,2,3}$ larger than corresponding widths of steady-state non-discretized flame (at least for models with well-localized flame profiles). Effects of discretization on flame profiles and propagation speed for model (3.2) were presented in Sec. 2.6; in part, flame speed agrees with steady state one up to $\sim 1\%$ when total flame width (from $f = 0$ to 1) was 16 zones or larger; better agreement is observed for smaller expansion.

When flame width is kept constant throughout the simulation (in units of grid spacing) it is preferable to use numerically found parameters $d$ and $w$ for discretized problem, specifically ones found numerically by modeling 1D flame with the same flame width as the one required for actual multidimensional simulation. This will correct for systematic discretization effect (its principal component, which manifested itself in 1D simulations resulted in $d$ and $w$ deviating from those for continuous, steady-state, model).

For direct numerical (non-steady) estimation of flame speed and width, as well as for almost all other numerical studies presented in this and the next chapters, dimensionally split piecewise-linear code ALLA (Khokhlov (1998, 2000)) was used. For all runs performed the fuel was taken as half $^{12}\text{C}$, half (by mass) $^{16}\text{O}$ mixture; real degenerate equation of state was used, gravity was set to zero. We assumed that the fuel transformed to nuclear statistical equilibrium composition (depending on local pressure) and all the heat released in the process was released within the “flame”. Physically this is not the case at lower densities in a WD (outer layers, $\rho \sim 2 \times 10^7 \text{ g cm}^{-3}$ and below), yet it is the expansion parameter $\Lambda$, dependence of flame characteristics on which we are interested in; all the results found are presented as functions of $\Lambda$, and not, say, of fuel density (this way, for any fixed $\Lambda$, they must be universal for any equation of state, providing assumptions of pressure and $H \rho$ being constant across the flame are satisfied). For SN Ia problem at lower densities it is thus straightforward to find corrections for our results: one just needs to use real heat release within the flame (slightly smaller than what we used, based on burning to NSE composition) to find correct value of expansion parameter $\Lambda$, and use our results (such as $d(\Lambda)$, $w(\Lambda)$, asphericity of flame surface in 3D, or Markstein number) for such found $\Lambda$. 
3.1.3 Results for flame profiles and velocities

Results of steady-state calculations of $d$ and $w$ for Models A (3.1–3.2), sKPP (3.3) and B (3.4–3.7) are presented in Table 3.1, together with the same quantities found numerically. As discussed above, the $d$ and $w$ found analytically, or by finding the eigenvalues and corresponding flame profile width through numerical integration of (2.2) (we call this “steady-state technique”, as opposed to direct numerical simulations, where physical quantities are discretized on computational grid), will yield correct prescribed flame speed $D$ and $W$ (when using (1.3) with parameters determined by (2.37) for “flame” evolution) only when $W$ is sufficiently large ($\sim 16$ cells or more, as tested for model A in Sec. 2.6). Systematic deviation from prescribed $D$ and $W$ grows as $W$ decreases. To correct for this deviation we numerically obtained $d_{\text{num}}$ and $w_{\text{num}}$ yielding correct prescribed $W_1$ and $D$. These depend on desired $W_1$ (tending to steady-state values as $W_1 \to \infty$), and should yield the required width and speed in 2D and 3D setting (as long as the front may be considered sufficiently flat, and providing its corresponding width is close to $W_1$ used to obtain $d_{\text{num}}$ and $w_{\text{num}}$ in 1D), with better accuracy than parameters $d_{\text{st}}$ and $w_{\text{st}}$ found through steady-state technique.

For model A $W_1$ was chosen so that to produce (almost total) width $W_3 = 6$, to use the results of Sec. 2.4, where simple analytical expressions were obtained for flame speed and total width ($f = 0$ to 1) for this model. For sKPP value $W_{1,\text{num}} = 4$ was chosen based on 2D performance: for smaller $W_1$ surface instabilities are too large at densities below $\sim 10^8$ g cm$^{-3}$. $W_1 = 3.2$ for model B provided reasonable performance for all densities studied, from $5 \times 10^9$ down to $8 \times 10^5$ g cm$^{-3}$. Flame speed required in simulations was $D = 80$ km s$^{-1}$, which is a reasonable value for laminar deflagration velocity near the center of a WD (Timmes & Woosley (1992)). In outer layers, at smaller densities, laminar deflagration speed decreases, yet one typically uses a value of “turbulent flame speed” $D \sim S_t \simeq 0.5\sqrt{A g \Delta}$ as prescribed $D$ there, which by far exceeds the laminar deflagration speed, due to large gravitational acceleration a fair distance from the star center ($A$ denotes Atwood number, Eq. 1.2).

Dependence of steady state dimensionless speeds $d$ and width $w_1$ on expansion parameter $\Lambda$ is further illustrated in Figs. 3.1–3.2. Shift parameter $\epsilon_a = \epsilon_f = 10^{-3}$ was used for sKPP model. The curves were rescaled to coincide at $1/\Lambda = 0$ (no expansion) to better represent the form of dependence on $\Lambda$. Absolute independent of $\Lambda$ normalizations are not of much interest for model use in simulations, as prescription (2.37) takes care of adjusting $\tilde{K}$ and $R$ for this. The form of the dependence on $1/\Lambda$, on the other hand, is more difficult to account for, and should be fitted on a model-by-model basis. Fig. 3.3 shows $w_3/w_1$ ratio as a function of expansion parameter. This ratio is an indicator of flame profile shapes. This ratio is larger for sKPP model (long tails in flame profile), which is a drawback, as the need to resolve the region where gradient of $f$ is large does not allow one to use flame model parameters $\tilde{K}$ and
| Model | 1/Λ | $d_{st}$ | $w_{1, st}$ | $w_{3, st}$ | $W_{1, \text{num}}$ | $d_{\text{num}}$ | $w_{1, \text{num}}$ | $w_{2, \text{num}}$ | $w_{3, \text{num}}$ |
|-------|-----|--------|------------|------------|-----------------|----------------|----------------|----------------|----------------|
| A     | 0.1670 | 1.498 | 1.225 | 1.837 | 3.56 | 1.424 | 1.209 | 1.819 | 2.035 |
| A     | 0.3980 | 1.411 | 1.289 | 1.919 | 3.48 | 1.333 | 1.268 | 1.897 | 2.198 |
| A     | 0.7337 | 1.306 | 1.376 | 2.030 | 3.44 | 1.222 | 1.351 | 2.000 | 2.358 |
| A     | 1.442 | 1.140 | 1.540 | 2.240 | 3.41 | 1.041 | 1.491 | 2.184 | 2.619 |
| A     | 8.571 | 0.5564 | 2.401 | 3.445 | 3.16 | 0.4304 | 2.014 | 2.888 | 3.830 |
| sKPP  | 0.1670 | 1.681 | 8.125 | 21.31 | 4.0 | 1.674 | 8.115 | 15.99 | 21.58 |
| sKPP  | 0.3980 | 1.664 | 8.893 | 23.39 | 4.0 | 1.596 | 8.585 | 16.86 | 22.82 |
| sKPP  | 0.7337 | 1.642 | 9.993 | 26.44 | 4.0 | 1.515 | 9.319 | 18.27 | 24.82 |
| sKPP  | 1.442 | 1.605 | 12.27 | 32.83 | 4.0 | 1.396 | 10.91 | 21.49 | 29.34 |
| sKPP  | 8.571 | 1.420 | 33.04 | 92.19 | 4.0 | 0.9592 | 22.76 | 46.77 | 65.00 |
| B     | 0.1670 | 0.3178 | 2.159 | 3.424 | 3.2 | 0.3121 | 2.147 | 3.441 | 4.145 |
| B     | 0.3980 | 0.2990 | 2.245 | 3.595 | 3.2 | 0.2921 | 2.236 | 3.583 | 4.310 |
| B     | 0.7337 | 0.1850 | 2.627 | 4.096 | 3.2 | 0.1751 | 2.553 | 4.058 | 4.842 |
| B     | 1.442 | 0.1221 | 2.865 | 4.455 | 3.2 | 0.1129 | 2.744 | 4.317 | 5.161 |
| B     | 8.571 | 0.0664 | 3.495 | 5.831 | 3.2 | 0.05816 | 3.119 | 4.920 | 6.016 |

Table 3.1: Steady-state flame speeds ($d_{st}$) and widths ($w_{1, st}$, $w_{3, st}$), compared to the ones found via direct numerical simulations. $W_1$ represents physical flame width in number of cells between $f = 0.9$ and $f = 0.1$ used in numerical estimates. $\rho_{\text{fuel}}$ corresponding to $1/\Lambda$ shown for a WD with 0.5C+0.5O composition are $2 \times 10^9$, $3 \times 10^8$, $10^8$, $3 \times 10^7$ and $8 \times 10^5$ g cm$^{-3}$ respectively. $D_{\text{num}} = 80$ km s$^{-1}$ for all the models. Shift parameters of sKPP model are $\epsilon_a = \epsilon_f = 10^{-3}$. 
Figure 3.1: Flame speed scaling as a function of expansion parameter $\Lambda$, found through steady-state technique for 3 models, A, B and sKPP with $\epsilon_a = \epsilon_f = 10^{-3}$. The speeds presented were rescaled by their respective values at zero expansion, $d_A(1/\Lambda = 0) = 1.5703$, $d_{sKPP}(1/\Lambda = 0) = 1.6954$, $d_B(1/\Lambda = 0) = 0.33335$. Non-monotonic dependence of $d_B$ on $\Lambda$ is due to burning rate dependence on expansion through nonmonotonic $c(\Lambda)$.

$R$ yielding too narrow $W_1$, and the total flame width then, illustrated by $W_3$ value is necessarily significantly larger for sKPP model than for models A and B.

For implementation in simulations using FC, Sec. 2.5.2, we fitted the dependence $d(\Lambda)$ and $w_1(\Lambda)$ for Model B. As parameter $c(\Lambda)$ in artificial reaction rate for Model B is defined as a spline, Eq. (3.7), the fit for speed and width is also given by different formulae on different intervals of $\Lambda$; it can be found in Appendix, Eq. (A.6).

These fits yield flame speed in 1D setting differing by at most 0.8% from required 80 km/s in a range $1/\Lambda \in [0.11; 8.6]$. Notice that as expansion increases dimensionless speed is expected to vanish $d(\Lambda) \propto \Lambda$, as it was the case for Model A; thus the fit should be modified (last part, at large expansions) if it is to be used at $1/\Lambda \gtrsim 8.6$.

### 3.2 Results for 1D numerical noises

As the flame propagates over the grid one would expect certain amount of acoustic noise generated. Because of discreteness of the grid there is no exact continuous translational invariance of the problem; say, total burning rate (in simulation), summed over grid zones in the flame region (where burning occurs) depends not only on continuous flame profile modeled, but on the precise positioning of that profile with respect to the grid as well. This leads to sound waves generation with period corresponding to time needed for the flame to move across one grid spacing. De-
Figure 3.2: Steady-state flame width $w_1 = \chi(f = 0.1) - \chi(f = 0.9)$ scaling as a function of expansion parameter $\Lambda$, for 3 models, A, B and sKPP with $\epsilon_a = \epsilon_f = 10^{-3}$. These widths are rescaled by their values at zero expansion, $w_{1A}(1/\Lambda = 0) = 1.1762$, $w_{1sKPP}(1/\Lambda = 0) = 7.5687$, $w_{1B}(1/\Lambda = 0) = 2.0924$.

Figure 3.3: Ratio of two dimensionless flame widths defined differently, $w_3/w_1$ ($w_3 = \chi|_{f=0.999}$, $w_1 = \chi|_{f=0.9}$, $\chi$ is a dimensionless flame coordinate) as a function of expansion parameter $\Lambda$, found through steady-state technique for 3 models, A, B and sKPP with $\epsilon_a = \epsilon_f = 10^{-3}$.
Figure 3.4: Flame profiles for models B and sKPP (black squares), $\rho_{\text{fuel}} = 3 \times 10^7 \text{g cm}^{-3}$, $1/\Lambda = 1.442$. Numerical profiles were recorded in 1D simulations at time step 5000. $W_{1sKPP} = 4$ and $W_{1B} = 3.2$ cells, the values used in multidimensional simulations. Steady state profiles (continuous line, shown only on the interval where $f_{st} \neq 0$ or 1.) were obtained by rescaling abscissas of steady profiles by $W_{1,\text{num}}/w_{1,\text{st}}$ (so that the rescaled profile width matched numerical one), and then translating in $x$ direction for best fit. Note long tails in sKPP profile.
pending on boundary conditions these waves may bounce back and forth, perhaps seeding and facilitating development of real physical instabilities of the system, thus complicating the simulation and making the results questionable. In this section we look at local physical quantities distribution in 1D domain (simulation tube), as well as time dependence of certain integral quantities, like burning rate.

All models are studied under the same conditions: same computation setup, quiet initial conditions (imitating steady state distribution of variables in simulation), flame speed is required to equal 80km s$^{-1}$ (which is achieved by choosing flame model parameters $\tilde{K}$ and $R$ as described in Sec. 3.1.1. Numerically found values for $d$ and $w$ for chosen numerical flame width were used). Flame widths are different for different models, but are required to be equal for each individual model for each run (unless specified otherwise) regardless of expansion parameter; these individual widths were chosen (for model B and sKPP) based on performance in 2D simulations (see next chapter), and are summarized, as $W_{1,\text{num}}$, in Table 3.1.

Flame speed as a function of integration time is presented in Fig. 3.5. It is apparent from the plot that while average in time flame speed is indeed equal to the prescribed value for all models, flame speed for model A fluctuates by more than 10% around the average, which is not a desired feature. Also note in this figure that transient effects due to not completely perfect initial conditions are completely relaxed for all models within 1200 integration timesteps, and that transient deviation in flame speed is within 3% for all models.

![Figure 3.5: Flame speed $D(t) = \frac{1}{\rho_{\text{fuel}}} \frac{d n_{\text{ash}}}{dt}$ as a function of integration time step. Fuel density is $2 \times 10^9$ g cm$^{-3}$.](image-url)
The pattern of fluctuations is presented in greater detail in Fig. 3.6 for expansion parameters typical in SN Ia problem at the beginning and closer to the end of burning in flamelet regime. Relative deviations from prescribed value was rescaled by a factor of 200 for model A there for it to have the same scale in the figures as the other models. The fluctuations are plotted against physical time, and the range of time shown for the two densities is inversely proportional to flame front speed with respect to grid, \( D(1 + 1/\Lambda) \). Thus the flame propagates through the same distance within the time shown for the two plots, approximately 8 grid spacings. And 8 periods of flame speed fluctuations are clearly seen in each figure, pattern of fluctuations in time is very similar for each period, but patterns for different models differ drastically.

![Graph showing relative flame speed fluctuations](image)

Figure 3.6: Relative flame speed \( D(t) \) deviation from its prescribed value \( D_0 = 80 \text{ km s}^{-1} \) as a function of time. Fuel density is \( 2 \times 10^9 \text{ g cm}^{-3} \) \( (1/\Lambda = \rho_{\text{fuel}}/\rho_{\text{ash}} - 1 = 0.1670) \) for the left figure, and \( 3 \times 10^7 \text{ g cm}^{-3} \) \( (1/\Lambda = 1.442) \) for the right one. For model A this deviation was divided by a factor of 200 so that the rescaled deviation had approximately the same scale as deviations for the other two models.

Next figures show distribution of physical variables in the tube at a fixed moment of time (timestep 5000). Matter densities and velocities are presented in Figs. 3.7–3.10. Sound waves are visible for all models superimposed on density and velocity jump across the flame. Their wavelength is the same for all models at a given density, and is different in the fuel and ash (as generation period is the same, but sound speed differs). Say, 6 wavelengths are visible in the figures at \( \rho_{\text{fuel}} = 3 \times 10^7 \text{ g cm}^{-3} \) in the fuel, between the flame and the right end of the tube. The pattern is complicated due to reflections off the boundaries. Reflections off the open (right) boundary were observed to be weak, which facilitates relaxation processes.
Figure 3.7: Distribution of density and matter velocity in the tube at timestep 5000 for model A. Fuel density is $3 \times 10^7$ g cm$^{-3}$. Note large fluctuations in matter velocity.

Figure 3.8: Density and matter velocity in the tube at timestep 5000 for model sKPP. Fuel density is $3 \times 10^7$ g cm$^{-3}$.

Figure 3.9: Density and matter velocity in the tube at timestep 5000 for model B, fuel density $3 \times 10^7$ g cm$^{-3}$. 
Figure 3.10: Density and matter velocity in the tube at timestep 5000 for model B, fuel density $2 \times 10^9$ g cm$^{-3}$.

Distribution of pressure is shown in Fig. 3.11. We show relative deviation from average pressure in the fuel: the latter is calculated by averaging over all cells where reaction progress variable $f < 10^{-4}$. Pattern of distribution of the pressure in the sound waves resembles that in density and velocity distributions. It is apparent that average pressure in the ash (left of the flame) is lower than that in the fuel (by $\sim \rho_{\text{fuel}} u^2 / c^2$, $c$ denoting sound speed). Also note a strong peak in the flame zone. Simulations with larger flame width, 20 cells and above, show several short pressure waves within the flame, with amplitude rapidly decreasing (as one leaves the flame; within a few zones) to the amplitude of pressure waves outside the flame zone; for models with step-function burning rate it is obvious from that pattern that pressure waves are generated in the cell where burning rate changes discontinuously. Heat starts releasing abruptly in the cell when $f$ value reaches $f_0$, generating strong pressure pulse. While exact numerical code used, boundary conditions, have effect on non-physical, numerical noise behavior in simulations, certain features in flame model have universal effect on noisiness of simulations where these models are used. These observations on noise generation show that models utilizing discontinuous burning rate functions are to produce significant noise. Table 3.2 quantifies our observations. On this grounds model A, with 10% fluctuations in flame speed as a function of time, and in matter velocity distribution in “steady” 1D flame propagation seems unacceptable for use in flame capturing.

Model B has continuous burning rate, which goes to zero as $f \rightarrow 0$ or 1. Burning rate (3.3) is also continuous, however there is a jump by shift parameter $\epsilon_f$ or $\epsilon_a$ when $f$ reaches 0 or 1, which must be a source of noise. Yet with values $\epsilon_f = \epsilon_a = 10^{-3}$ this jump is $\sim 1000$ times smaller than in model A (or original model, Khokhlov (1995)); as a result 1D noises are comparable for sKPP and model B. We concentrate on studying these 2 models further on.
Table 3.2: Numerical noise in 1D simulations. Each $\epsilon$ written needs to be multiplied by $10^{-4}$ to yield actual relative dispersion. Average flame speed was 80 km s$^{-1}$, flame width as in Table 3.1 ($W_1 = 3.2$ cells for model B, 4 cells for sKPP, $W_3 = 6$ cells for A), except 2 entries for model A, for which $W_3 = 24$ cells. Note that making flame wider for model A still does not render noises acceptable. Simulation box was 256 cells long for expansion parameter $1/\Lambda < 1.5$ and 2048 cells long for larger expansion. For each run dispersion of $D(t)$ was found over $N = 8000$ steps from 2001 to 10000, its relative value $\epsilon_D = \sqrt{\langle D^2(t) \rangle_t - \langle D(t) \rangle_t^2} / \langle D(t) \rangle_t$ is shown (here $\langle \ldots \rangle_t$ stands for averaging over the $N$ timesteps). $\epsilon_p$ represents relative dispersion in pressure in the fuel averaged over time: at each timestep relative dispersion of pressure in the fuel was calculated, $\epsilon_p(t) = \sqrt{\langle p(x)^2 \rangle_f - \langle p(x) \rangle_f^2} / \langle p(x) \rangle_f$; $\langle \ldots \rangle_f$ means taking average in space over fuel cells, defined as cells where progress variable $f < 0.0001$; these $\epsilon_p(t)$ were than averaged over $N = 8000$ last timesteps to yield $\epsilon_p$ shown in the table. $\epsilon_{u,\text{ash}}$ represents relative dispersion in matter velocity in the ash in the same manner: at every timestep $\epsilon_{u,\text{ash}}(t) = \sqrt{\langle u(x)^2 \rangle_a - \langle u(x) \rangle_a^2} / \langle u(x) \rangle_a$ was defined ($\langle \ldots \rangle_a$ meaning averaging over cells with ash, where $f > 0.9999$); these were averaged over the 8000 timesteps to yield $\epsilon_{u,\text{ash}}$ shown.

| Model | $1/\Lambda$ | $\epsilon_D$ | $\epsilon_{u,\text{ash}}$ | $\epsilon_p$ | Model | $1/\Lambda$ | $\epsilon_D$ | $\epsilon_{u,\text{ash}}$ | $\epsilon_p$ |
|-------|-------------|---------------|----------------|--------------|-------|-------------|---------------|----------------|--------------|
| B     | 0.167       | 4.39          | 1.72           | 0.0237       | sKPP  | 0.167       | 2.24          | 0.577          | 0.00794       |
| B     | 0.398       | 2.28          | 6.69           | 0.154        | sKPP  | 0.398       | 2.22          | 1.55           | 0.0358        |
| B     | 0.734       | 1.91          | 12.03          | 0.421        | sKPP  | 0.734       | 2.25          | 3.18           | 0.111         |
| B     | 1.44        | 6.38          | 21.1           | 0.79         | sKPP  | 1.44        | 2.9           | 25.6           | 0.95          |
| B     | 2.33        | 5.83          | 18.4           | 2.07         | sKPP  | 2.33        | 3.85          | 13.9           | 1.52          |
| B     | 5.05        | 14.6          | 10.7           | 3.26         | sKPP  | 5.05        | 10.6          | 10.4           | 3.18          |
| B     | 8.57        | 21.5          | 70.4           | 45.1         | sKPP  | 8.57        | 17.1          | 120            | 85.2          |
| A     | 0.167       | 726           | 69.6           | 0.958        | $A, W_3 = 24$ | 0.167       | 167           | 15.8           | 0.226         |
| A     | 1.44        | 733           | 225            | 14.2         | $A, W_3 = 24$ | 1.44        | 228           | 64.3           | 4.06          |
Figure 3.11: Distribution of relative pressure deviation (from its mean value in the fuel $p_0$) in the tube at timestep 5000. Fuel density is $2 \times 10^9 \text{g cm}^{-3}$ in the left figure, and $3 \times 10^7 \text{g cm}^{-3}$ in the right one.
CHAPTER 4
FLAMES IN 2D AND 3D SIMULATIONS

In addition to numerical noises that manifest themselves in 1D as well, there are two physical phenomena that should affect flame propagation in more than one dimensions. First, normal flame speed of a curved flame generally depends on the front curvature. This is usually called Markstein effect, though this term also refers to specific form of that dependence, namely flame speed depending linearly on flame curvature:

\[ D_R = D_R = \infty \left( 1 - \frac{Ma}{R} \right) \]

\( R \) here denotes radius of curvature of the flame; \( D_R \) stands for normal propagation speed of a flame with radius of curvature \( R \); proportionality parameter \( Ma \) is called Markstein length. Such linear dependence was observed in experiments and simulations (Markstein (1964)). See next chapter for more detail, and for studying this effect numerically on model flames.

Second, when fuel and ash densities are different, Landau-Darrieus (LD) instability leads to growth of small perturbations on smooth flame surface, resulting in wrinkling the flame, and formation of corners later on. Perturbations of any wavelength are unstable in idealized case of infinitely thin flame with no Markstein effect (Darrieus (1938); Landau (1944)), that is when flame speed does not depend on curvature. When \( Ma > 0 \), for infinitely thin flame, only perturbations with wavelength exceeding certain critical value \( \lambda_{cr} \) grow. This is what is observed for all our models. Besides Markstein length found positive, the flame width is significant (\( \sim 4 \) cells, comparable to initial radius of burnt bubble in simulations). Theory of LD-type instability of finite-thickness flames is much more involved (see, e.g. Matalon & Matkowsky (1982)). It can be expected that the critical wavelength exceeds a few flame widths; its exact value, as well as instability growth rate should depend on exact distribution of density and heat production within the flame. Numerical effects may additionally distort flame surface. The aim of this section is to study how the shape of initially spherical bubble changes with time.

4.1 Simulation setup

As for 1D simulations of Chap. 3 we use uniform grid with the same grid spacing across all our simulations. The simulations were run in square \( N \times N \) cells box in 2D, cubic \( N \times N \times N \) box in 3D; \( N \) ranging from 64 (box side 132 km) to 2048 (4224 km) for 2D simulations, and from 64 to 256 for 3D ones. Normalizations \( \tilde{K} \) and \( \tilde{R} \) of flame model diffusivity and reaction rate are chosen, as in 1D simulations described above, via (2.37), to yield “flame” speed 80 km \( s^{-1} \) and width \( W_1 \) as shown in Tab. 3.1, unless specified otherwise.

For all simulations one of two types of boundary conditions is used. In first type of simulations deflagration is initiated by a sphere of hot ash placed fully in the interior of the square/cubic grid (except for a few runs described below initial flame
center coincides with box center); outflow boundary conditions are imposed on all boundaries. Initial distribution of reaction variable $f$ and physical quantities is set smooth, corresponding to quasi-steady state spherical flame burning outward. Initial conditions are characterized by initial spherical “flame” center position $(x_0, y_0)$, and radius $R_0$; the latter signifies here radius of the surface $f = 0.9$. Explicitly, abscissa of 1D steady-state flame profile $f(\chi)$ (steady progress variable as a function of dimensionless coordinate, eigenfunction of (2.8)) is rescaled so that flame width ($f = 0.1$ to $f = 0.9$) were $W_1$ (the width of the flame we want to achieve) and then translated; in precise terms $f(\chi) \mapsto c(r) : c(r) = f \left( (r - r_0) \frac{W_1}{W_1} \right)$, translation $r_0$ chosen such that $c(R_0) = 0.9$. Initial reaction progress variable distribution is then set spherically symmetrically around the center of what we loosely call “a sphere of burned material at $t = 0$”, according to this rescaled profile $c(r)$, $r$ being a distance from the flame center. So, if the center of some cell is $R_0$ from the flame center, initial value of reaction progress variable is 0.9 in that cell; if it is $R_0 + W_1$ off the center, progress variable is 0.1 there, etc. $f$ is zero for all cells more than total flame width away from the initial “sphere of ash”, and is 1 at the center of that sphere (unless the flame is too wide, and its tail reaches the center). Other thermodynamical variables, and matter velocity are distributed accordingly, mimicking their distribution for quasi-steady state spherical flame burning outward from the center (though neglecting the difference in flame profile $f$ of spherical and planar flame).

Simulations of second type are run in quadrant (2D) or octant (3D): burning is initiated from the corner of the cube, by filling a sector of a sphere centered at that corner with ash. As for the full cube simulations, this wording means smooth initial distribution of thermo- and hydrodynamical variables mimicking quasi-steady state 2D/3D burning from the corner, with reaction variable $f(r = R_0) = 0.9$ and $f(r = R_0 + W_1) = 0.1$ at $t = 0$; matter velocity directed radially off the ash sector vertex (in computation cube corner), matter resting at the corner. Reflecting boundary conditions are imposed (throughout the run) on 2 sides/3 faces crossing in that corner, and outflow boundary conditions on the rest of simulation box sides/faces. Such quadrant/octant simulations are more economical and must provide the same results as full cube simulations, thanks to the problem symmetry about the cube center when central ignition is used. These are customarily used in literature for this reason. Quite severe numerical artifacts are often observed in such octant simulations, with system behavior along octant reflecting faces significantly different from bulk behavior. We use both types of setup precisely to check how different results one gets in full-cube and octant simulations, due to, say, LD instability seeding (or mod-

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1. full cube containing 4 times more cells in 2D, 8 times more in 3D; due to symmetry all 8 full-cube octants behave the same, and presumably the same way as one isolated octant with reflecting boundary conditions on 3 faces passing through its vertex.
ification) by the boundaries, or maybe just imperfectly realized boundary conditions — in our simpler setting, with simple chemistry and without gravity.

4.2 Flame behavior in 2D, theory and observations

Fig. 4.1 shows how initially spherical flame evolves with time, for the 3 models studied with expansion parameter $1/\Lambda = 1.442$ ($\rho_{\text{fuel}} = 3 \times 10^7 \text{ g cm}^{-3}$). One can observe two features of flame evolution: first, some global anisotropy develops, it looks like flame propagates faster along axes than along the diagonal of the grid, for Model A and sKPP; second, small scale wrinkling of the flame surface is observed, resembling LD instability development. It is seen that Model sKPP, despite having largest width $W_1$ (and by far largest $W_3$) demonstrates the largest distortion of spherical surface as deflagration progresses. The fact that Model A behaves better shows that these 2D distortions are unrelated to 1D noises, by far strongest for Model A. This rules out possible explanation of 2D behavior by relating it to flame speed fluctuations in time, different in different directions. Pressure waves due to numerical noise are by far most intensive for Model A in 2D/3D as well, yet these waves are also not the most important factor in disturbing flame surface, as comparison of flame surfaces for the models demonstrates.

These observed phenomena are detrimental for use in flame capturing. Of course, real flame region is subject to its own instabilities, it interacts with real physical sound waves and turbulence; all of these distort its surface, initially spherically flame will quickly become non-spherical in real world, as our model flames do. However, the fact that the amount of distortion strongly depends on the model, even for comparable “flame” widths (making any flame thinner aggravates asphericity development, so when sKPP model width is made to match that of Model B its behavior becomes further worse) shows that there is no hope that some random model instability development would miraculously match that of real physical flame region. Anisotropy in flame speed is clearly a numerical artifact and is not observed in nature. There is no control over small scale wrinkles developing on “flame” surface (apart from making the “flame” wider; see results below). Therefore the best model is clearly the one preserving spherical flame surface as closely as possible, and this is how model B was designed.

Evidence below suggests that small-scale perturbations have the nature of LD-instability. It is then understandable that actual distribution of matter density within the “flame” in part, influences smallest unstable scale $\lambda_{\text{cr}}$, as well as instability growing rate, which naturally explains why different models behave differently. From the figures below it follows that sKPP has the smallest $\lambda_{\text{cr}}$, and instabilities grow fastest. Models A and B yield flames having density distribution within the flame closer to linear, this seems to make them more stable to LD-like instability. As observed in Khokhlov (1995) approximately linear density distribution is also the...
Figure 4.1: Flame for the 3 models, represented by surfaces where reaction variable $f = 0.5$. Coordinates are in units of box size, e.g. $x = \pm 0.5$ corresponds to right/left boundary. Fuel density is $3 \times 10^7$ g cm$^{-3}$. The outermost surface is that of Model B, at timestep 14000, when flame radius is $R = 22R_0$; initial radius $R_0 = 30$ km for all runs shown in this Figure. This flame is also shown at earlier time, when its radius is $9R_0$. Innermost circle represents flame surfaces at $t = 0$. For Model sKPP surfaces are shown (thick solid lines) for timesteps when $R = 7R_0$ and when $R = 18R_0$. Note that global asphericity due to anisotropic flame speed is the most prominent feature at early times, and at later times small-scale LD-type instabilities severely distort flame surface. Dotted line shows flame position for Model A when its radius $R = 20R_0$. 
case for real flame zone (averaged over scales corresponding to typical numerical grid sizes) in RT-driven deflagration simulations, in SN Ia simulations in part. Hence there is more hope that Model B (and not sKPP) would behave more similar to real flame region in terms of flame perturbations evolution.

Fig. 4.2 shows flame surface for model B in simulations in quadrant $1024 \times 1024$ cells at late times, when radius is large enough to exceed minimal unstable perturbation length, and enough time has passed for the instability to develop. In this figure small-scale surface features evolution, seen in Fig. 4.1 for Model sKPP, looks like typical LD instability development. Notice that, as expected, characteristic length of perturbations increases with fuel density, as expansion across the flame decreases. In Fig. 4.1, at $1/\Lambda = 1.442$ just first signs of instability development can be seen, with length of order of a quarter of the flame circumference, $\sim 400$ cells. Thus, even though at any density flame with large enough radius will become LD unstable, for densities $\rho_{\text{fuel}} \gtrsim 3 \times 10^7 \text{g cm}^{-3}$ time required for instability development exceeds typical multidimensional simulation durations. More careful quantitative analysis shows (some numbers are presented below) that there is not much difference between quadrant and full-square runs (ones with central ignition) in terms of surface perturbations as long as flame arc length in quadrant does not exceed a few $\lambda_{\text{cr}}$, characteristic lengths of LD-type perturbations. After that boundaries do contribute to instability growth in their vicinity, yet for the durations our runs had (enough for the flame to pass $\sim 1000$ cells) there was not seen apparent difference far enough from the axes for full-square and quadrant simulations (for Model B). This may be seen for a few runs shown in Fig. 4.2.

At smaller expansions all models behave better in 2D, no asphericity is seen by naked eye in simulations with fuel density of above $3 \times 10^8 \text{g cm}^{-3}$ ($1/\Lambda < 0.4$; some quantitative results are presented in the next subsection). At larger expansions, however, sKPP flames behavior deteriorates rapidly, making sKPP model use in FC dangerous at physically interesting densities (down to a few times $10^6 \text{g cm}^{-3}$, although there is less time for instability development at smaller densities, as corresponding regions are reached later in simulations with ignition close to star center). When sKPP model shift parameters $\epsilon_a$, $\epsilon_f$ are increased the flame becomes more stable to LD-type instability (being another piece of evidence suggesting that long sKPP profile tails may be related to predisposition to LD instability for sKPP model: these tails are shorter for larger parameters $\epsilon_a$, $\epsilon_f$); global flame anisotropy is not improved significantly with increasing flame parameters. 1D noises become objectionable at larger shifts, reaching, e.g. 1.8% average dispersion in flame speed at $\epsilon_a = \epsilon_f = 0.1$, $1/\Lambda = 1.442$ (0.54% at $\epsilon_a = \epsilon_f = 0.03$, 0.38% at $\epsilon_a = \epsilon_f = 0.01$). Values $\epsilon_a = \epsilon_f = 10^{-3}$ yield 1D noises close to those for Model B (at corresponding flame widths we use); sKPP is studied with these $\epsilon_{a,f}$ values below, unless indicated otherwise. There might be a hope that making sKPP flames slightly wider could drastically improve their stability. As Fig. 4.3 shows, LD-like instability is
really suppressed for wider flames, expectedly; however, global flame propagation anisotropy decreases rather slowly with increasing flame width. Hence we are forced to conclude that for use at larger expansions, $1/\Lambda \sim 0.6$ and larger, Model B is the only viable candidate of all the models we considered.

### 4.3 Numerical results for flame shape evolution, 2D

Here we trace how flame shape changes with time for models B and sKPP, for a range of fuel densities. Besides comparing model to model in similar conditions we also want to compare flame asphericity development for different initial flame radius, and for different distances to the boundaries. By varying initial radius we want to better understand the role of initial conditions, whether instabilities readily grow from the very beginning of the computation (and then this growth will be further accelerated in astrophysical simulations with gravity), or whether there is some initial interval of time when flame radius is small and LD-type instabilities decay (then, in part, unavoidable imperfections of initial conditions will not play that significant role in flame behavior at later times, which is desirable); what the dependence of global flame propagation anisotropy on flame radius is. To check the role of boundaries on flame surface evolution we compare behavior of the models at different resolutions; while keeping grid spacing the same this effectively moves boundaries further away from flame surface, whereas flame width and initial radius remain fixed, both in terms of number of cells and in physical units.

In Table 4.1 flame geometry is characterized by 2 numbers (called flame asphericity parameters below). First, by interpolation we find a set of points $(r_i, \phi_i)$ (in polar coordinates) on the surface $f = 0.5$. Among these we find the two with extremal distances from flame center $r_{\text{max}}$ and $r_{\text{min}}$, average radius over all points, $R = \langle r_i \rangle$, and the best fit of $r_i$ distribution with $\tilde{r}_i = r_0 + r_1 \cos 4\phi_i$. The two numbers we use to describe flame surface are $\Delta r/R = (r_{\text{max}} - r_{\text{min}})/R$ and $r_1/r_0$ (All values written in Tab. 4.1 are multiplied by a common factor of $10^3$.) These numbers give rough idea about flame surface: if it is circular both numbers are zero; if $r_1/r_0$ is close to one half of $\Delta r/R$ one would conclude that large-scale anisotropy of flame propagation speed is the main feature, dominating over amplitudes of small-scale LD-type wrinkling; if $r_1/r_0$ is significantly less than one half of $\Delta r/R$ the wrinkles yield more contribution into $\Delta r/R$ than systematic large-scale anisotropy of flame surface.

As observed in the previous section, flame shape in figures, for Model sKPP $r_1/r_0 > 0$, flame surface is in average closer to its center along diagonal of the grid than along grid axes. For Model B this systematic anisotropy is controlled by parameter $c(\Lambda)$ in the burning rate. If, at a given expansion, term $c(\Lambda)$ is used that is larger than its optimal value (which we approximate as $(3.7)$) the flame propagation speed along grid diagonal exceeds that along grid axes, and vice versa; this anisotropy is related to dependence of density distribution within the “flame” on $c(\Lambda)$ (governing
Figure 4.2: Flame surface for Model B at late times, for high expansion, corresponding to fuel densities $8 \times 10^5$, $5 \times 10^6$ and $10^7$ g cm$^{-3}$. For each density two flame positions are shown (indicated by flame radius written next to corresponding surface, in km): when perturbations by LD-type instabilities start to be visible, and when they are well developed. Notice that characteristic lengths of perturbations increase as expansion across the flame decreases; also that the flame retains reasonably spherical shape (globally) until late enough times: $R = 540$ km is the same as the radius of SKPP flame in Fig. 4.1. Initial radii of the flames were $R_0 = 120$ km for $1/\Lambda = 2.33$, $R_0 = 90$ km for $1/\Lambda = 3.18$, $R_0 = 30$ km for $1/\Lambda = 8.57$. For $1/\Lambda = 8.57$ results of one more simulation are shown (one flame surface when its radius reached 900 km, short dash). This simulation was run in full square (with central ignition; only one quadrant is shown, $x = 0.5$ corresponds to simulation box boundary for this last surface, whereas $x = 1$ is right box boundary for rest of the runs), initial radius $R_0 = 240$ km. It is apparent from comparison that characteristic lengths scales of surface perturbations are determined solely by expansion, and do not show any significant correlation with initial radius. No large scale structure anisotropy of flame surface is visible for the central ignition run, even though its surface shown is just 15% of the box size off the box boundary. Finally, at times shown there is not much difference between large scale anisotropy for central and corner ignition; it is more noticeable at later times, and perturbations generation on reflecting boundaries can be seen, but overall the difference between quadrant and full-square runs is not large (for Model B) until so late times when open boundaries start playing a role (this was checked for full-square simulations in up to $2048 \times 2048$ boxes for some densities).
Figure 4.3: Flame surface for Model sKPP with $W_1 = 4, 8$ and 16 cells, $\rho_{\text{fuel}} = 3 \times 10^7$ g cm$^{-3}$. One quadrant of full-square simulation ($1024^2$) is shown; $x = 0.5$ represents right boundary of the box. Solid line represents $f = 0.5$ curve in a $W_1 = 4$ flame when its average radius is 600 km. Dotted line shows the curve defined the same way for $W_1 = 8$ flame when its radius reached 630 km. Dashed line shows $W_1 = 16$ flame with radius 660 km. Note that LD-type wrinkles are fully developed for $W_1 = 4$ flame, but for $W_1 = 16$ flame just first signs of instability development are seen at the radius shown; lengthscale of the wrinkles increases with flame width. Also note that the flame is still noticeably closer to the center along grid diagonal than along the axes even for $W_1 = 16$. 
reaction rate distribution within the “flame”). The values we suggest in (3.7) were chosen this way, to optimize flame speed anisotropy.

It was checked in simulations with different resolutions that boundaries start playing a role in disturbing flame surface when the flame passes approximately half way from the center to box boundary face. Numbers $\Delta r/R$ and $r_1/r_0$ at that point start deviating from those observed in the runs with larger box (in terms of number of cells; the flames have the same width, and are compared at the same radius for smaller and larger boxes), by a factor of order 1.4–2, indicating that actual perturbation started developing somewhat earlier, and have grown to an extent such that deviations in flame asphericity parameters become significant.

Asphericities summarized in Tab. 2.3 suggest that the role of boundary conditions is under control, and seemingly the same for Model B and sKPP, and whether the flame is stable or not. Numerical noises in the bulk, far from the flame surface are comparable for models B and sKPP, all this evidence suggests that it is not some intricate interaction with boundaries which makes sKPP flame speed anisotropic, but rather local properties of sKPP flame. Small scale ripples generation may be more susceptible to background noises in sKPP model, this partly explaining fast growing amplitudes of those. Regardless of whether there is any significant contribution to wrinkle growth due to waves reflected from the boundaries, Model sKPP is unsuitable for simulations with large expansions of matter across the flame. For clarity, nonetheless, we performed several runs with off-center ignition to verify whether instability growth is mostly governed by local physics near the flame, or whether better boundary conditions may, to extent, improve sKPP flames behavior. In those full-square runs initial conditions corresponded to quasi-steady spherical 2D burning, with flame center not coinciding with the center of the cube. Results for flame centered at points $(0; 0.2)$ and $(0.1; 0.1)$ (in units of box size: $x = \pm 0.5$ are two of the box boundaries in these units) for expansion $1/\Lambda = 1.44$ are shown in Tab. 4.1 together with results for central ignition. It is seen that asphericity parameters do not differ drastically for these 3 setups. Same holds true for smaller expansions, when asphericities are less, as well as for Model B. Fig. 4.4 shows flame surfaces for the 3 setups: small scale wrinkles look very similar, regardless of relative distances to the boundaries.

In the next section we present some results for growth or decay of a sinusoidal perturbation on a planar 2D flame. Those quantitatively confirm that the small-scale instability we observe on circular flames are really of LD type. This suggests that the results should not qualitatively depend on a particular code used for simulations, as they are a manifestation of a real physical phenomenon, which should be observed with any code. Large scale flame speed anisotropy, as we saw, depends to some extent on flame width, it is likely to depend on a particular way derivatives are estimated by the code (larger stencils used would have effect of additionally smearing the flame, thus stabilizing it to some extent), yet the qualitative result that diagonal
Table 4.1: Asphericity of flame surface at different times, for models B and sKPP. Each $\frac{\Delta r}{R}$ shown needs to be multiplied with a factor $10^{-3}$ to yield actual $\frac{\Delta r}{R}$; same for $r_1/r_0$. Each pair of asphericity parameters is shown for 4 different moments in time, when flame surface radius reached $R_1 = R_0 + 30$ (km) (the 1st pair of columns), $R_2 = R_0 + 90$ (the 2nd pair), $R_3 = R_0 + 270$ (the 3rd pair), and $R_5 = R_0 + 600$ (the last one). Unless specified otherwise each model is assumed to yield $D = 80$ km s$^{-1}$, and width $W_1$=3.2 cells for Model B, and 4 cells for sKPP. Initial flame radius $R_0 = 30$ km (unless different $R_0$ is specified; $R_0$ and $R$ are in kilometers in this Table.) Default setup is central ignition, 1024$^2$ grid cells; simulations in quadrant with corner ignition are indicated by letter “q” at model name; if the side of a simulation box is different from $N = 1024$ grid cells, actual $N$ is specified next to model name. For default $R_0 = 30$ km the moments of time shown roughly represent moments when boundary conditions start playing a role for central ignition simulations in boxes with sides 128, 256, 512 and 1024 cells respectively (this corresponds to the time when flame surface is about its radius away from the boundaries; this is true regardless of whether the flame is LD-unstable or not (at radii shown), as may be seen on the results in the Table for Model sKPP at $1/\Lambda \geq 0.734$ or Model B at $1/\Lambda \geq 2.33$.

| Model      | $1/\Lambda$ | $\frac{\Delta r}{R}$ | $r_1/r_0$ | $\frac{\Delta r}{R}$ | $r_1/r_0$ | $\frac{\Delta r}{R}$ | $r_1/r_0$ | $\frac{\Delta r}{R}$ | $r_1/r_0$ |
|------------|-------------|-----------------------|-----------|-----------------------|-----------|-----------------------|-----------|-----------------------|-----------|
| sKPPq, $N = 512$ | 0.167       | 1.36                  | 0.787     | 3.42                  | 1.38      | 5.45                  | 2.76      | 8.40                  | 4.19      |
| sKPPq       | 0.398       | 2.16                  | -1.23     | 3.07                  | -1.65     | 3.34                  | -1.12     | 1.58                  | 0.083     |
| Bq          | 0.398       | 2.93                  | -1.74     | 8.61                  | -4.80     | 11.8                  | -5.96     | 11.4                  | -5.59     |
| sKPP        | 0.734       | 8.57                  | 4.00      | 19.8                  | 9.87      | 29.4                  | 11.4      | 49.0                  | 18.7      |
| B, $N = 512$ | 0.734       | 3.12                  | 0.331     | 5.42                  | 1.60      | 8.06                  | 1.34      | -                    | -         |
| Bq, $N = 512$| 0.734       | 2.37                  | 0.246     | 5.28                  | 1.49      | 9.85                  | -2.33     | 11.8                  | -1.88     |
| sKPP        | 1.44        | 13.3                  | 4.79      | 54.6                  | 24.5      | 99.2                  | 36.4      | 197                   | 53.6      |
| sKPP, $W_1 = 8$ | 1.44       | 7.09                  | 2.03      | 37.5                  | 17.1      | 41.9                  | 19.4      | 60.9                  | 23.8      |
| sKPP, $W_1 = 16$ | 1.44     | 3.58                  | -0.988    | 26.1                  | 10.2      | 36.5                  | 13.5      | 47.2                  | 17.0      |
| sKPP, $\epsilon = 0.01$ | 1.44     | 6.41                  | 1.62      | 30.0                  | 14.1      | 39.6                  | 13.2      | 79.3                  | 22.2      |
| sKPP, $\epsilon = 0.03$ | 1.44     | 3.63                  | -0.811    | 16.0                  | 6.40      | 13.5                  | 4.37      | 34.9                  | 3.63      |
| sKPP, $x_0, y_0 = 0.1$ | 1.44     | 14.6                  | 5.21      | 50.6                  | 23.9      | 96.4                  | 30.8      | 204                   | 55.0      |
| sKPP, $y_0 = 0.2$ | 1.44     | 11.6                  | 4.23      | 57.1                  | 22.5      | 116                   | 32.1      | 314                   | 33.5      |
| B           | 1.44        | 8.17                  | -4.58     | 2.77                  | 0.59      | 3.75                  | -1.17     | 8.80                  | 0.046     |
| B, $R = 90$ | 1.44        | 6.86                  | -3.64     | 9.47                  | -4.51     | 12.1                  | -5.68     | 11.0                  | -3.11     |
| B, $R = 180$| 1.44        | 4.03                  | -1.78     | 7.89                  | -3.61     | 9.69                  | -4.41     | 11.9                  | 4.31      |
| B, $R = 15$ | 1.44        | 7.61                  | 3.69      | 17.6                  | 9.43      | 8.78                  | 3.79      | 9.57                  | 3.24      |
| Bq, $N = 512$| 1.44        | 7.93                  | -4.68     | 2.66                  | 1.09      | 2.93                  | -1.08     | 7.89                  | 0.14      |
| B, $R = 90$, $N = 2^{11}$ | 2.33   | 12.3                  | -6.23     | 18.2                  | -9.20     | 23.5                  | -9.35     | 50.5                  | -10.5     |
| B, $R = 90$ | 2.33        | 12.4                  | -6.23     | 17.9                  | -8.93     | 26.5                  | -9.25     | 48.6                  | -1.86     |
| B           | 2.33        | 20.0                  | -11.7     | 15.8                  | -7.09     | 18.5                  | -3.92     | 34.9                  | 0.09      |
| B, $R = 90$ | 3.18        | 14.1                  | -6.76     | 20.3                  | -10.6     | 24.7                  | -11.9     | 43.0                  | -12.3     |
| B           | 8.57        | 4.31                  | -2.22     | 6.68                  | -2.95     | 12.7                  | -5.05     | 34.6                  | -5.69     |
Figure 4.4: Flame surface for Model sKPP with different locations of a seed flame at $t = 0$. $\rho_{\text{fuel}} = 3 \times 10^7 \text{ g cm}^{-3}$, $D = 80 \text{ km s}^{-1}$, $W_1 = 4 \text{ cells}$, $R_0 = 30 \text{ km}$, each flame is shown when its radius reached 360 km (at timestep about 7500). Dashed line shows the flame with central ignition, $x_0 = y_0 = 0$ (box boundaries are at $x, y = \pm 0.5$); solid line corresponds to the flame with $x_0 = y_0 = 0.1$, and dotted one to the flame with $x_0 = 0, y_0 = 0.2$. Notice that the first signs of large-scale distortions are seen on the flame closest to the boundary, due to matter speed asymmetry, yet small scale perturbations on all three flames show essentially the same amplitude.
propagation is slower than that along the axes (for sKPP) is likely to hold true for any code. It would be interesting to systematically check our results with a different numerical scheme. While we have not performed systematic code-to-code comparison, typical results obtained with code ALLA were confirmed with FLASH code (Fryxell et al. (2000)), for Model sKPP developing global asphericity and LD-type instabilities with short unstable length, and Model B showing much better behavior in this respects at lower fuel density. Derivatives are estimated with 4th order accuracy in FLASH code (vs 2nd order in ALLA). Fig. 4.5 shows a typical flame surface simulated in quadrant 256 × 256 with FLASH code, with the same flame model parameters as discussed above, with 1/Λ = 1.44. Same features of the model are observed.

![Flame surface](image)

Figure 4.5: Flame surface for Model sKPP, ρ_{fuel} = 3 \times 10^7 \text{ g cm}^{-3}, D = 80 \text{ km s}^{-1}, W_1 = 4 \text{ cells}, computed in quadrant 256 \times 256 \text{ cells with } \text{FLASH code.}

### 4.4 Perturbed planar 2D flames, LD instability

Here we present results of a study of the instability development on sinusoidally-perturbed planar flames in 2D. We simulate such flames in rectangular domains with reflecting boundary conditions on 3 of the sides, and outflow boundary condition on the fourth side, towards which the flame propagates. We observe that for domains with a width below certain critical value L_{cr} (which depends on expansion parameter and the flame model used) the perturbation decays as the flame propagates. For wider
domains certain non-planar flame surface develops, which steadily propagates into the fuel.

4.4.1 Theoretical background

The behavior we observe, flames in wide domains developing non-planar front shape, qualitatively agrees with known from experiments behavior of terrestrial flames; however, no analytical studies have been done in the regime relevant in FC, with fairly wide flames and non-negligible expansion of matter across the flame.

First theoretical studies of this type of instability, linear analysis of its development (when the perturbation is small), were done by Landau (1944) and Darrieus (1938) in approximation of infinitely thin flame, with flame velocity independent of its geometry and background hydrodynamical flows; the result is that perturbations with any wave number $k$ grow exponentially, with the rate $\omega$ proportional to $k$:

$$\omega_{LD}(k) = kD\frac{-\sigma + \sqrt{\sigma^3 + \sigma^2 - \sigma}}{\sigma + 1}. \quad (4.1)$$

$D$ here denotes flame speed, $\sigma = \rho_{\text{fuel}}/\rho_{\text{ash}} = 1/\Lambda + 1$. As discussed above this approximation is invalid at small perturbation lengths, comparable with the flame width. Real flames are generally stable with respect to such short-wavelength perturbations.

A simple (and physically sound) modification of the original LD consideration leading to stable perturbations with large enough $k$ is to take into account flame speed dependence on the flame curvature. Assuming linear dependence on curvature $1/R$, $D(R) = D_{R=\infty} \left(1 - \frac{Ma}{R}\right)$, still in the limit of infinitely thin flame, modified dispersion relation is given by (Markstein (1964))

$$\omega = \frac{kD}{\sigma + 1} \left[-\sigma(1 + Ma k) + \sqrt{\sigma^3 + \sigma^2 - \sigma + (Ma k - 2\sigma)Ma k\sigma^2}\right]. \quad (4.2)$$

For positive $Ma$, which is the case for all flame models we consider for FC applications and for most chemical flames in practice, perturbations with

$$2\pi/k < \lambda_{cr}(Ma) = 4\pi(\Lambda + 1)Ma \quad (4.3)$$
decay. This is understood qualitatively, as positive $Ma$ stabilizes the flame by decreasing propagation velocity on convex parts of the flame surface (the ones that are

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2. $Ma$ may be negative in, e.g., systems with significantly different diffusivities of different reactants when the most diffusive reactant is deficient (for example for lean hydrogen-oxygen flames), cf. Matalon et al. (2003) for theoretical study. Infinitely thin flames with negative $Ma$ are unstable for any perturbation wavelength, as are flames in original LD approximation, with $Ma = 0$. 

displaced forward into the fuel, with respect to a plane unperturbed flame surface), and increasing the propagation velocity into fuel on concave parts, which are behind the unperturbed surface. This effect tends to suppress growth of the instabilities (due to main component of LD instability, with $D(R)$ dependence neglected), and it does stabilize the smooth flame surface at sufficiently short perturbations (when curvature is larger, and this curvature effect is more pronounced).

Linear analysis was also performed up to the first order in flame width (in Matalon & Matkowsky (1982); Pelce & Clavin (1982); Matalon et al. (2003), under different conditions), thus elucidating the effect of flames being not infinitely thin, and obtaining some estimates for Markstein lengths. These works only deal with Arrhenius-type reaction rates, thus the results are not directly applicable to our flame models; besides, especially for sKPP, the “flame” width is quite close to observed minimal unstable wavelength, thus the first order terms in asymptotic expansion in small $Wk$ are not apriori likely to provide a trustworthy description of instability development\(^3\). According to our simulations (summarized below) the critical width of the tube, at which stable regime of flame propagation changes from planar front to certain nonlinearly stabilized shape, closely corresponds to an estimate based on Eq. (4.3) for model B; this quantitative agreement proves that the small-scale instability we observed in 2D in the previous section is of the hydrodynamic, LD-type nature.

### 4.4.2 Numerical results, comparison to theoretical estimates

Results for critical tube side $L_{cr}$ orthogonal to flame propagation, its smallest value at which initial perturbation develops into certain nonplanar shape (instead of relaxing to planar surface, which happens at smaller $L$), are summarized in Tab. 4.2. We used 512 cells long computation domains for larger expansions, corresponding to fuel densities in a 0.5C+0.5O WD of $10^8$ g cm\(^{-3}\) and below, and 2048 cells long domains for smaller expansions; initial perturbation was one sine wave on the domain width for most of the runs, with amplitude equal to $0.1L$. Initial distribution (in the flame propagation direction) of progress variable $f$ and physical quantities corresponded to 1D steady flame profiles. For larger expansion, $1/\Lambda \geq 1.44$, uncertainty in $L_{cr}$ is about 2 cells, the smallest amount by which we could change the tube side; the smallest supercritical width observed is shown in the table. At these larger expansions

\(^3\) Markstein numbers, which are the ratios of Markstein lengths and corresponding flame widths, are typically between $-1$ and 6 for chemical flames, according to the cited theoretical estimates, and to experimentally found values. Markstein numbers for our model flames are between 0.2 and 0.5 for Model B (larger values corresponding to larger expansion), and about 3 times smaller for Model sKPP with $\epsilon_a = \epsilon_f = 10^{-3}$ (and go to zero as sKPP shift parameters $\epsilon_a, \epsilon_f$ go to zero.) See next chapter for more detail.
the steady flame shape significantly deviates from planar (see Fig. 4.6 for example), and the critical tube width is easy to recognize.

| $1/\Lambda$ | 0.167 | 0.249 | 0.398 | 0.734 | 1.44 | 2.33 | 3.18 | 3.95 | 5.05 | 8.57 |
|------------|-------|-------|-------|-------|------|------|------|------|------|------|
| $\lambda_{cr}(Ma)$ | 60.3 | 43.4 | 30.6 | 30.8 | 30.0 | 19.7 | 19.0 | 18.8 | 18.7 | 19.3 |
| $L_{cr}^*$ | 68 | 48 | 32 | 34 | 32 | 24 | 26 | 20 | 16 | 16 |
| $L_{cr}^*/5, W_1 = 16$ | | | | | | | 17.6 | 16.0 | | |

Table 4.2: Minimal tube width (in cells) at which planar flame is hydrodynamically unstable, at different expansions $1/\Lambda$. $\lambda_{cr}(Ma)$, the 2nd row, is a theoretical prediction (4.3) in Markstein approximation (of infinitely thin flame, with linear Markstein law for flame speed dependence on the front curvature); the values of Markstein length were taken from Tab. 5.1. The third row shows estimates of the critical tube width from above from direct numerical simulations (evolution of initially sinusoidal front in 2D tube); these are the smallest values we found to yield non-planar (non-linearly stabilized) steadily propagating flames. The estimate from below is 2 cells smaller for $1/\Lambda \geq 1.44$, and 4 cells smaller for the lower expansions shown. Flame speed is 80 km s$^{-1}$, flame width $W_1 = 3.2$ cells. The last row shows same upper estimates for $L_{cr}^*$ obtained for $W_1 = 16$ cells wide flames ($V = 80$ km s$^{-1}$), to understand whether somewhat different relation between $L_{cr}^*$ and estimate $\lambda_{cr}(Ma)$ at higher expansion represents a physical effect (corresponding to increased role of finite flame width), or numerical discretization effect (observed in Sec. 2.6 to be more pronounced at larger expansion, for various quantities). This latter $L_{cr}^*$ was divided by 5, so that to offset the effect of Markstein length $Ma$ (and thus corresponding $\lambda_{cr}(Ma)$) being 5 times larger for this extra wide “flame”.

For smaller expansion, on the other hand, nonlinearly-stabilized non-planar shape at near-critical tube width only deviates by a few cells from the plane, for tube widths of tens of cells. This deviation scales approximately as $1/\Lambda$ when this expansion parameter is $\ll 1$, in accord with analytical studies (Sivashinsky (1977); Michelson & Sivashinsky (1977)), this making recognition of critical tube width less certain. Besides, relaxation times become significantly longer at smaller expansion: linear growth rate in LD approximation scales as $0.5Dk/\Lambda$; Eq. (4.2) yields growth rate scaling $\propto 1/\Lambda^3$ (assuming $Ma$ going to some constant value at zero expansion) near critical tube width $L_{cr} = \lambda_{cr}(Ma)$ (4.3): $\omega_{Ma}(L_{cr} + \delta L) = \frac{D \delta L}{16\pi Ma^2 \Lambda^3}$. The newest version of the code allowing stable computation for over 300000 timesteps required for densities of $2 \times 10^9$ g cm$^{-3}$ and above became unavailable to us in the middle of this study, thus uncertainties for $\lambda_{cr}$ at smaller expansions are estimated to be of order 4 cells. Only one run was finished at fuel density $5 \times 10^9$ g cm$^{-3}$ ($1/\Lambda = 0.118$, $\lambda_{cr}(Ma) = 82$ cells); the domain width of 72 cells was found subcritical.

It is interesting to observe agreement within about 10% between numerically found values for the critical tube width and theoretical estimate in Markstein approxi-
Figure 4.6: Perturbed planar flame evolution at $1/\Lambda = 1.44$ for subcritical $L = 30\Delta$ and supercritical $L = 32\Delta$ domain width. $x$ and $y$ are in units of the domain length, which is 512 cells; $y$-scale is the same for both $L$. Flames are shown at timesteps 0, 7000 and 14000. The flame at $t = 7000$ was translated by $-0.25$ in $x$-direction, the one at $t = 14000$ was translated by $-0.5$, to show all three on the same plot.

Information at expansions (1.44 and below), corresponding to fuel density of $3 \times 10^7 \text{g cm}^{-3}$ in SN Ia problem. It is even better at expansions $1/\Lambda < 0.734$ if Markstein numbers found in direct numerical simulations (see Tab. 5.1) are used. At higher expansion agreement is somewhat worse. The fact that at smaller expansions observed $L_{cr}$ is somewhat larger that theoretical one may be attributed to numerical diffusion tails in $f$ profiles, thus yielding somewhat larger Markstein length than the one found in continuous quasi-steady state technique. At smaller expansions, however, numerically estimated $L_{cr}$ becomes smaller than $\lambda_{cr}(Ma)$. To check whether we understand the effect of “flame” discreteness properly we reran some simulations at small densities with distinct normalization of the “flame” governing parameters, $\tilde{K}$ and $R$, to yield “flames” with 5 times larger width, for which the effects of discreteness must be less pronounced. As Markstein length (and thus $\lambda_{cr}(Ma)$) scales proportionally to the flame width we divided observed upper estimate $L_{cr}^*$ for such wider flames by 5, for direct comparison with the rest of the numbers in the table. The effect of changing the flame width is significant (as it was for other quantities related to the “flame” in Sec. 2.6 at large expansions), yet in the predicted direction: critical perturbation length decreases when discretization effects become smaller. Thus we are tempted to conclude that the discrepancy observed at higher expansions is due to real physical deviation from Markstein approximation, due to finite flame width (moreover, representing a larger fraction of $L_{cr}$ at these larger expansions); this deviation seems to monotonically increase with expansion.
For model sKPP with $\epsilon_a = \epsilon_f = 10^{-3}$ and $W_1 = 4$ cells the critical perturbation wavelength is about 2.5 times smaller at small expansions (in Markstein approximation — as are corresponding Markstein lengths, cf. Tab. 5.1 for Markstein numbers). These are even smaller at larger expansions, 7 times smaller than those for Model B at $1/\Lambda = 1.44$. We really observe steadily propagating non-planar sKPP flames (corresponding to a full wavelength, not reorganizing into a half-wave configuration) in domains 10 cells wide at $\rho_{\text{fuel}} = 3 \times 10^7$ g cm$^{-3}$, 8 cells wide at $\rho_{\text{fuel}} \leq 5 \times 10^6$; $L_{cr} \approx 8$ at $\rho_{\text{fuel}} = 10^7$ — a seemingly stable non-planar configuration in 8 cells wide domain starts transforming into a half-wave configuration after running through 120 cells (this flame relaxes to a stable half-wave configuration when it runs through 250 more cells). Flame profile, $f$ distribution across the flame, in such stationary flames is clearly distorted; the flame is wider where it is convex towards the fuel. At smaller expansions $L_{cr}$ is noticeably larger than according to Markstein approximation, say it is 30 cells at $\rho_{\text{fuel}} = 3 \times 10^8$ g cm$^{-3}$, almost the same value as for Model B (with standardly used for the latter $W_1 = 3.2$ though, i.e. thinner than the sKPP flame).

4.4.3 Discussion

Steady flame shapes we observe in supercritically wide domains visually resemble the ones reported in Rastigejev & Matalon (2006), the only study we are aware of dealing theoretically/numerically with non-linear stabilization of flames with finite expansion. Results for flame shapes are compared there to analytical results of Michelson & Sivashinsky (1977) for small expansion, with convincing agreement. Methodology of Rastigejev & Matalon (2006) is quite different from ours: the authors try to study non-linear stabilization in Markstein approximation, with infinitely thin flame (tracked with Level Set technique), Markstein effect introduced by hand in prescribing flame speed as a function of locally computed curvature. Results for critical wavelength are not reported there with reasonable accuracy, although for a few expansions it is noted whether existence of stable non-planar shape is in agreement with linear stability analysis, Eq. (4.3). Our observations agree with those in Rastigejev & Matalon (2006) in that the most stable flame shape has exactly one maximum for supercritical tube width; this also agrees with analytical results in small expansion case$^4$.

$^4$ These observations do not seem conclusive though. Say, our results might suggest that a configuration with several wavelength corresponding to a stably propagating flame shape, arranged end-to-end on a tube width, may be stable with respect to sufficiently small perturbations. Such configurations were obtained by starting with several sinusoidal wavelengths on a tube width as an initial condition; this evolved to described configuration, rather that to one-maximum one; this configuration in several runs propagated (quasi-)stably through entire 2048-cell long domain. Moreover, certain small perturbations not respecting the discrete symmetry of multi-wave configuration seemed to decay, without transforming the multwave configuration into an absolutely stable one with one maximum on tube width. In other runs, however, with superficially similar initial condi-
We used reflecting boundary conditions on long boundaries of the computation domain, whereas Rastigejev & Matalon (2006) use periodic ones. This makes it possible for us to observe another stable propagation mode, different from that shown in Fig. 4.6, namely, the one with a half of the steady flame shape occupying the whole tube width. Such a mode is expected to be more stable than the one with the whole profile (symmetric with respect to the longitudinal symmetry axis of the tube). However the times needed for transition from a (quasi-)stable whole-wavelength shape to stable half-wavelength shape, with just numerical noises in our simulations as a trigger, were usually long; only in a few runs could we observe such a transition, in tubes with width not sufficient to support a stable non-planar profile with one wavelength, but wide enough to accommodate a half of the critical wavelength. Since this happened more readily at larger expansions, for some of the corresponding results we report in Tab. 4.2 we used asymmetric initial conditions, with half of a sine wave on tube width (maximum on one side, minimum on the other).

To sum up, results of this section show that the small-scale instability we observed in 2D simulations is indeed a hydrodynamic instability of LD-type. It is masked for Model sKPP with numerical artifacts, like global flame propagation anisotropy, and demonstrates significantly different characteristic instability lengthscales and growth rates in different directions. For Model B numerical artifacts are almost absent, and characteristic for LD instability shapes are easily recognized on 2D flames.

Dominating lengthscales of perturbations of cylindrical flames show somewhat stronger dependence on expansion parameter than observed above critical wavelengths of perturbations on planar flames (we refer to Model B through the end of this section). The weak dependence of the latter is in accord with linear results in Markstein approximation: Eq. 4.3 suggests rather weak dependence of $\lambda_{cr}$ at expansions $1/\Lambda \geq 2.33$: dependence through factor $1 + \Lambda$ (weak at small $\Lambda$) is further offset with (accidentally?) correlated dependence $Ma(\Lambda)$. Theoretical (linear) results for LD-type instability for spherical flames (see, e.g., Zeldovich et al. (1985), Ch. 6) in Markstein approximation help to qualitatively understand characteristic lengthscales of the perturbations, as well as timescales associated with their developments (each wave having supercritical length, in part) perturbations started to grow asymmetrically, with the shape transforming to a one-wave or a half-wave configuration. Rastigejev & Matalon (2006) started with random flame shape, with no symmetries, in simulations dedicated to getting one-wave configuration in the process of instability developing towards its nonlinear stabilization; thus no results are presented to judge about local stability of multi-wave configurations. This is in contrast to analytical results in small-expansion analysis, where instability of any configuration distinct from a one-maximum one is proven mathematically. Those results, however, are obtained for basically a different problem, with all terms beyond first order in $1/\Lambda$ dropped (similarly to our estimates for $d(\Lambda)$ based on expansion in $1/\Lambda$ at the end of Sec. 2.3.2). It is plausible that for the full problem there may be islands of stability in perturbation space near multiwave-configurations, vanishing as $1/\Lambda \to 0$, or perhaps islands existing only when finiteness of the flame width is taken into account. This requires further study.
development. In contrast with nonlinear stabilization of flames in the tube, where the stable shape (at least in the limit of small expansion) steadily propagating has a maximum, for spherical flames only higher harmonics are unstable; the ones represented by spherical functions $P_m^n(\cos \theta)e^{i m \phi}$ with index $n$ less than certain critical value grow slower than the flame expands, and do not lead to the surface distortion as time progresses (all harmonics grow according to a power law in 3D and 2D, not exponentially as perturbations on a planar flame). This critical index is $n_{cr} = 12$ for positive Markstein length and $1/\Lambda \approx 3$. For larger and smaller expansion the critical index is larger.

For any supercritical harmonic $n$ a perturbation having corresponding distribution over the flame surface will grow after the flame has reached certain radius $r(n)$. Markstein effect will not inhibit growth of any supercritical harmonic at late enough times, as the linear size of corresponding perturbation scales proportionally to the flame radius, and will eventually become large enough for Markstein stabilizing effect to become non-substantial. The harmonic that becomes unstable at the smallest flame radius will dominate for some time, however we are not aware of any theoretical studies for characteristic perturbations structure at late times. According to flame surfaces in Fig. 4.2 for the times studied linear perturbation lengthscales stay approximately constant with time, cells expanded with the flame keep subdividing into smaller cells. Characteristic linear perturbation scale is about 50 cells for $1/\Lambda = 8.57$, and larger for smaller expansions, according to the figure. Ratio of this scale to $\lambda_{cr}$ for planar flames is about 3 at this expansion, and somewhat larger at smaller expansions.

To reiterate, theoretical results we summarized correspond to a spherical flame in 3D in Markstein approximation, thus specific numbers, like $n_{cr}$, first harmonic to start growing, etc. are not expected to describe well results of our simulations of cylindrical flames in the previous section. Qualitative picture, however, presented in the previous paragraph seems to apply to 2D as well as 3D setup (following the derivations in 3D), and agrees with the features of small-scale instability development we observed in numerical simulations. One particularly interesting number to check is a critical radius of the flame when the first unstable mode appears. According to linear analysis in 3D in Zeldovich et al. (1985) this radius is $r_{cr} = Ma \tau^*$, where dimensionless $\tau^*$ depends on expansion, and is about 60–70 for $1/\Lambda \in [2.33; 8.57]$, about 80 for $1/\Lambda = 1.44$, 120 for $1/\Lambda = 0.734$, 300 for $1/\Lambda = 0.398$, > 600 for $1/\Lambda = 0.167$. For $1/\Lambda = 1.44$ this yields $r_{cr} \approx 110$ cells, or 230 km; this seems to reasonably well agree with numerical results in 3D we present in the following section.
4.5 3D results for flame shape evolution

LD-type wrinkling of flame surface is expected to grow faster in 3D and may become an issue for Model B at larger expansions; it is likely to remain a problem for Model sKPP.

Our approach is the same as described for 2D simulations. Flame propagation is initiated either from the center of the cubic computation box with outflow boundary conditions on all faces, or from the corner, with reflecting boundary conditions on the 3 faces passing through that corner, and outflow boundary conditions on the other three faces; we refer to the latter setup as a simulation in octant. Initial distribution of physical variables and reaction variable $f$ is spherically symmetric around the flame center; a sphere (a sector for octant simulations) around the center contains hot ash of the reaction at rest; away from the initially burned region physical variables correspond to fuel, moving radially outwards, according to quasisteady solution for a spherical flame in 3D; in the intermediate region, the “flame” itself, physical quantities correspond to a mixture of fuel and ash, $f$ has some intermediate value monotonically changing from 1 in the burned sphere to 0 in the fuel ahead of the flame, according to 1D steady-state profile. The distance from the initial “flame” center to the point where $f = 0.9$ is called initial flame radius $R_0$.

The largest computational box we use for 3D simulations is $256^3$; LD-type instabilities do not have enough time to develop to the extent close to that in 2D simulations. To characterize flame geometry we use several numbers akin to those we used in the previous section. First, $\Delta r/R$ (defined the same way as for 2D, by dividing the difference $\Delta r$ between extremal radii on $f = 0.5$ surface by the average distance $R$ from the flame center over all points on the surface) characterizes overall sphericity. To get an idea about large scale deviations from the spherical shape, and in which directions these are maximal, we consider cross-sections of $f = 0.5$ surface by equatorial plane ($z = 0$), by planes containing $z$ axis and forming angle $\pi/4$ or $\pi/8$ with $xz$ plane, and finally by 2 planes parallel to $xy$ plane, $z = R/2$ and $z = R\sqrt{3}/2$. We mark results for these planes with index 0, 4, 8, 2 and 3 respectively. For each plane we consider a slice, subset of points on the surface $f = 0.5$ that are at most $R/10$ away from the crossing plane. For points on each slice we compute fit parameters $r_0$ and $r_1$ similarly to what we did for 2D flames. For instance, for plane 2, parallel to $xy$ plane, we fit cylindrical coordinates ($\rho_i = \sqrt{x_i^2 + y_i^2}, \phi_i$) of points in the corresponding nearby slice with $\tilde{\rho}_i = r_{02} + r_{12}\cos 4\phi_i$.

The ratios $r_1/r_0$ for the slices described are listed in Tab. 4.3 for models B and sKPP for several densities, for several moments of time for each density; these ratios give an idea about flame surface geometry. Moments of time shown were chosen as in the previous section. We remind that, according to 2D comparisons, open boundaries start influencing results for flame surface, for $256^3$ runs, when its radius
reaches approximately 120 km (about 60 cells) for central ignition, and approximately 300 km for corner ignition (octant simulations).

| Model     | $1/\Lambda$ | $R$ | $\Delta r/R$ | $r_{10}$ | $r_{14}$ | $r_{18}$ | $r_{12}$ | $r_{13}$ |
|-----------|-------------|-----|---------------|----------|----------|----------|----------|----------|
| Bo, $N = 128$ | 0.167 | 120 | 8.81 | -3.24 | -2.12 | -2.56 | -4.14 | 3.94 |
| Bo, $N = 128$ | 0.167 | 195 | 6.37 | -2.10 | -1.41 | -1.65 | -2.84 | 1.92 |
| Ko, $N = 128$ | 0.167 | 195 | 7.87 | 3.71 | 1.73 | 2.56 | 2.34 | -8.99 |
| sKPP     | 0.398 | 120 | 6.22 | -1.24 | -1.73 | -1.66 | -1.97 | 4.76 |
| sKPP     | 0.398 | 210 | 7.53 | 3.23 | 0.77 | 2.08 | -0.78 | 4.33 |
| sKPP     | 0.734 | 60  | 27.4 | 4.34 | 9.88 | 5.59 | 10.9 | -7.62 |
| sKPP     | 0.734 | 120 | 55.3 | 12.5 | 18.1 | 10.4 | 20.7 | 4.07 |
| sKPP     | 0.734 | 195 | 75.6 | 15.9 | 24.8 | 15.1 | 27.6 | 5.02 |
| B        | 0.734 | 60  | 17.0 | 0.27 | 7.01 | 1.39 | 5.69 | 1.11 |
| B        | 0.734 | 120 | 32.3 | 2.82 | 13.4 | 4.48 | 16.5 | 7.32 |
| B        | 0.734 | 195 | 43.0 | 6.10 | 15.9 | 6.24 | 17.5 | 15.9 |
| Bo, $N = 128$ | 0.734 | 120 | 31.7 | 2.94 | 13.3 | 3.90 | 16.9 | 7.51 |
| Bo, $N = 128$ | 0.734 | 195 | 42.0 | 6.11 | 15.8 | 5.59 | 16.9 | 8.76 |
| sKPP     | 1.44  | 60  | 34.9 | 6.17 | 9.42 | 7.41 | 9.48 | 5.16 |
| sKPP     | 1.44  | 120 | 118 | 23.8 | 25.9 | 23.9 | 46.0 | 14.9 |
| sKPP     | 1.44  | 195 | 75.6 | 15.9 | 24.8 | 15.1 | 27.6 | 5.02 |
| Bo       | 1.44  | 60  | 14.1 | -5.14 | -1.78 | -3.49 | - | -0.8 |
| B        | 1.44  | 120 | 31.9 | 3.59 | 7.57 | 4.23 | - | 0.99 |
| B        | 1.44  | 195 | 46.7 | 10.7 | 10.7 | 9.63 | - | 36.9 |
| B, $R_0 = 90$ | 1.44 | 195 | 13.8 | 3.26 | 2.26 | 2.08 | 1.73 | -0.36 |
| B        | 1.44  | 120 | 13.1 | -4.60 | -1.29 | -3.07 | 1.19 | -11.0 |
| Bo       | 1.44  | 120 | 29.2 | 3.73 | 7.02 | 4.18 | 11.2 | 7.96 |
| Bo       | 1.44  | 195 | 30.9 | 3.42 | 7.22 | 3.93 | 12.4 | 7.30 |
| Bo       | 1.44  | 300 | 31.9 | 3.25 | 7.35 | 3.11 | 14.3 | 2.54 |

Table 4.3: Asphericity parameters, multiplied by 1000, at different times (indicated by radius $R$ the flame has reached), for models B and sKPP (abbreviated to K in some places) in 3D. Flame velocity is $D = 80 \text{ km s}^{-1}$, width $W_1=3.2$ cells for Model B, 4 cells for sKPP. Default initial flame radius is $R_0 = 30 \text{ km}$, box size $256^3$ (side 528 km), central ignition by default. If other than default values were used, they are indicated next to the model name; octant simulations are indicated by letter “o”.

As in 2D simulations, when expansion is small, $1/\Lambda < 0.4$, both models behave well, asphericity parameters stay within 1% even when flame surface is close to box boundaries. According to theoretical estimate in Markstein approximation, quoted in the previous section, first unstable modes start growing at flame radius exceeding 200 cells at such expansions (for Model B), and growth rate is small at small expansion. Already at $1/\Lambda = 0.734$, corresponding to fuel density $10^8 \text{ g cm}^{-3}$ in SNIa problem.
(with half carbon, half oxygen fuel) asphericity parameters grow almost linearly with time for both models, although even extremal $\Delta r/R$ remain within 5% for model B (as they do for this model for $1/\Lambda = 1.44$). One can observe that $r_1i$ is positive and grows for all times shown for model B, in contrast to the behavior for 2D simulations. It is noteworthy that for Model B results for octant and full-cube simulations are quite close to each other, with somewhat worse agreement for cross-section 3 (explicable, as flame surface forms sharp angle with crossing plane in this section, thus small 3D perturbations would look larger in the section). This implies that reflecting boundaries do not alter significantly LD instability of adjacent flame surface, thus octant simulations may be reliably used for modeling SNe Ia with central ignition (as far as “flame” propagation anisotropy and LD instability are concerned).
CHAPTER 5
MARKSTEIN EFFECT

In numerical simulations of flame propagation in 2D and 3D we observed that the instantaneous flame speed was somewhat different from the one measured for 1D flame in a tube with the same diffusivity and burning rate in governing equation (1.3). It was smaller at the beginning of the simulation (at least for small expansion); Markstein effect is a possible physical explanation of this phenomenon. Flame front is stretched by geometrical effects when it is not planar; density and velocity distribution across such a curved flame differ from those in planar steady flame, as a result so does instantaneous normal propagation speed. On general grounds one might expect corrections to flame propagation speed for small curvatures as expansion

$$D_{r_0} = D_{r_0=\infty} \left(1 - \frac{Ma}{r_0} + \frac{Ma_2}{r_0^2} + \ldots\right)$$

for the speed $D_{r_0}$ of a flame with radius of curvature $r_0$ in inverse powers of (large) $r_0$. In 3D this expansion could be more involved, with two principal radii of curvature of the flame surface $r_{01}, r_{02}$ appearing on the right hand side. Such systematic deviation of the speed of the curved flame from planar one was observed in experiments (see Markstein (1964)); the leading term, $Ma/r_0$ is enough to account for curvature corrections in those. In 3D setting $1/r_0 = 1/r_{01} + 1/r_{02}$ must be used in the term linear in curvature (the only linear combination invariant under rotations).

Negative sign at $Ma/R$ in (5.1) was chosen for convenience: with such a convention $Ma > 0$ for our model flames; some authors use notation with all pluses in (5.1). Notation $Ma_2$ (as well as $Ma_3$ and so on for coefficients of next terms in expansion (5.1)) is ours, such corrections of higher order in curvature are not studied in the literature.

In this chapter we study this curvature effect, first in quasi-steady state approach we describe, and then numerically for the flame models presented in the previous chapter. We compare the results obtained using these 2 methods, and conclude that for model B physical Markstein effect dominates numerical effects, as well as corrections to effective flame propagation speed due to hydrodynamic instability development at expansions of $1/\Lambda = 1.44$ and below.

5.1 Quasi-steady state technique

Here we present a general method for obtaining Markstein lengths of diffusion-reaction flames. No assumptions of small reaction zone thickness are made (unlike existing studies; for the model flames we consider, and are interested to apply the technique for, “preheating” and “reaction” zones have the same spatial scale). For
a spherical flame corresponding quasi-steady velocity (slowly changing with time as the flame radius changes) is found as an eigenvalue of a set of differential equations for quasi-steady distribution of matter velocity and quantities governing reaction rates (species concentrations and the temperature for physical combustion systems, reaction progress variable \( f \) for the model flames we considered before). Results for model flames are presented in the next sections.

For clarity we present the method for a system with reaction rate dependent on concentration of one species \( f \) and on temperature \( T \) (a typical approximation in studying premixed flames in chemical and astrophysical simulations). For convenience we suppose reaction rate \( \Phi = R\Phi_0 \) represented as a function of enthalpy density \( H \) instead of the temperature. Neglecting viscosity the system is described by Euler equation for matter velocity \( u \),

\[
\frac{\partial u}{\partial t} + (u \nabla) u = -\frac{\nabla p}{\rho} + g, \tag{5.2}
\]

mass continuity equation for evolution of the density \( \rho \) distribution

\[
\frac{\partial \rho}{\partial t} + \nabla (\rho u) = 0 \tag{5.3}
\]

and the following equations describing species diffusion and thermal conduction:

\[
\frac{\partial f}{\partial t} + u \nabla f = \nabla (K \nabla f) + R\Phi_0(f, H) \tag{5.4}
\]

\[
\frac{\partial H}{\partial t} + u \nabla H = \nabla (\kappa \nabla H) + qR\Phi_0(f, H). \tag{5.5}
\]

Here \( q \) represents specific heat release of the reaction. \( K = \tilde{K}K_0(f, H) \) is diffusivity of the species described by variable \( f \), \( \kappa = \tilde{\kappa}\kappa_0(f, H) \) is heat diffusivity; form-factors \( K_0, \kappa_0 \) and \( \Phi_0 \) are dimensionless. We assume \( f \) normalized as for the model flames of the previous chapters, namely \( f = 0 \) corresponding to unburned fuel, and \( f = 1 \) to reaction product (say, a state with deficient reactant completely depleted). No external volume force \( \rho g \) is supposed to be present below. We consider isobaric burning regime (quasi-steady deflagration with matter velocities much smaller than the sound speed), as we did in Chap. 2.

For model flames with reaction rate dependent on reaction variable \( f \) only the system is simplified, in the same way as it is simplified in the case of unit Lewis number \( Le \) (see below); essentially, Eq. (5.5) decouples from the rest of the system. With several species taken into account in reaction rates the needed modifications are also straightforward: an extra equation of type (5.4) is added to the system for each additional species; to the final eigenvalue problem (see below, (5.7–5.9) 2
ordinary first-order equations are added for each such species, no new complications are introduced.

The system of combustion equations has a solution describing a spherical flame propagating outwards. It approximately describes deflagration in a system consisting of pure fuel at rest at \( t = 0 \) and ignited at one point, after certain quasi-steady distribution of matter velocity and thermodynamic quantities is established, on timescales comparable to sound crossing time of the system. Such centrally symmetric distributions \( (f(r), \text{etc.}) \) propagate with the flame, changing slowly due to geometry (flame radius) changing — in contrast to a planar flame there is no exact translational symmetry (in \( r \)) for such a system, thus no steady solutions in the strict sense. We refer to system behavior like this as quasi-steady spherical flame propagation — when all quantities depend only on the distance from the flame center and time, and their changing with time in the frame coexpanding with the flame, that is expanding with so defined instantaneous flame velocity \( D(t) \), is much slower than in the rest-frame. For any quantity \( (f, \rho, H, \text{radial matter velocity } u_r, \text{etc.}) \) in coexpanding coordinates \( (r, t) \mapsto (\eta, t) \), \( \eta = r - \int D(t) dt \) partial time derivatives are small at fixed location \( \eta \) with respect to expanding flame surface. For corresponding time derivatives in laboratory coordinates \( (r, t) \)

\[
\left. \frac{\partial f}{\partial t} \right|_r = \left. \frac{\partial f}{\partial t} \right|_\eta - D(t) \left. \frac{\partial f}{\partial \eta} \right|_t \approx - D(t) \left. \frac{\partial f}{\partial \eta} \right|_t, 
\]

(5.6)
that is the changes due to profiles slowly reorganizing with changing geometry are negligible in comparison with changes due to flame propagation. We rewrite the system (5.2–5.5) below in comoving quasisteady coordinate \( \eta \) thus getting rid of explicit time dependence (it will enter only implicitly through flame radius \( r_0 \) dependence on time) based on approximate equality like (5.6) holding for \( \rho, H, u_r \). Such a substitution for time derivatives yields the eigenproblem, which determines the quasi-steady flame propagation speed \( D \) we seek for.

In dimensionless variables

\[
\tilde{\eta} = \eta \sqrt{R/K} \\
\tilde{r} = r \sqrt{R/K} \\
\tilde{u} = u_r / \sqrt{RK} \\
\tilde{d} = D / \sqrt{RK} \\
\tilde{H} = H / q \\
\lambda = \tilde{\kappa} / K
\]
after quasi-steady substitution of the form (5.6) equations (5.3–5.5) are rewritten as

\[(\hat{u} - d) \frac{d \rho}{d \tilde{\eta}} = -\rho \tilde{r}^{-\alpha} \frac{d}{d \tilde{\eta}}(\tilde{u} \tilde{r}^\alpha)\]  
(5.7)

\[(\hat{u} - d) \frac{d f}{d \tilde{\eta}} = \frac{d}{d \tilde{\eta}} \left( K_0 df \right) + \frac{\alpha K_0 df}{\tilde{r}} \frac{d \tilde{r}}{d \tilde{\eta}} + \Phi_0(f)\]  
(5.8)

\[(\hat{u} - d) \frac{d \tilde{H}}{d \tilde{\eta}} = \lambda \left[ \frac{d}{d \tilde{\eta}} \left( \kappa_0 d \tilde{H} \right) \right] + \Phi_0(f)\]  
(5.9)

In the above \(\alpha + 1 = \) dimension of the problem: \(\alpha = 1\) for a cylindrical flame, \(\alpha = 2\) for a spherical flame \((S^2)\) in 3D. Using corresponding equation of state and assumed isobaricity one expresses \(\rho\) as a function of \(\tilde{H}\) in Eq. (5.7), thus making the system closed. We used \(\rho = \text{const}/H\) as we did in the previous chapters.

Boundary conditions for this problem we use are

\[\tilde{r} = \tilde{r}_0 \equiv r_0 \sqrt{R/K} : \ f = 1, \ df/d\tilde{\eta} = 0, \ d\tilde{H}/d\tilde{\eta} = 0, \ \hat{u} = 0;\]  
(5.10)

\[\tilde{r} \to +\infty : \ f \to 0, \ H \to H_0/q \equiv H(P_{\text{fuel}}, T_{\text{fuel}})/q.\]  
(5.11)

It is through these boundary conditions that the flame radius \(r_0\) enters the eigenproblem, thus yielding its eigenvalue \(d\) dependent on \(r_0\). In prescribing boundary condition at \(r = r_0\) we assumed that the flame does not have infinite tail into ash. Formulation of quasi-steady problem for systems with such an infinite tail encounters several problems, we will not touch them here.

As in 1D case the system simplifies when \(\kappa = K\) \(i.e.\) Lewis number equals 1; we see, below, that these equal transfer coefficients may still depend arbitrarily on \(f\) and \(H\) for the simplification to hold; \(Le \approx 1\) in terrestrial flames, in nearly ideal gases). In this case we just reproduce a known result (Zeldovich & Frank-Kamenetskii (1938)) that distributions of \(f\) and \(H\) is similar — for any flame geometry (not necessarily spherical): Eq. (5.5) in this case coincides with (5.4) after rescaling \(H\) by \(q\), and boundary conditions (for \(f\) and \(H\) going to constants behind and in front of the flame) then yield algebraic relation \(H = H_0 + qf\); one is left with a reduced system of equations (5.3–5.4). The same simplification occurs in the case of model flames studied for Flame Capturing applications, when \(H = H_0 + qf\) is postulated by the technique.

We present results for \(D(r_0)\) in the next section, for model flames studied in the Chap. 2.
5.2 Quasi-steady results for models used in Flame Capturing

Below we stick to a reduced form of the eigenvalue problem, with $H = H_0 + qf$. $\rho H = \text{const}$ at constant pressure is assumed. Although the system (5.7–5.8) is not translationally invariant in $\tilde{r}$ (unlike the case for a planar front) due to $\tilde{r}$ explicitly appearing, $\tilde{r}$ does not change significantly within the flame width at large radii. For numerical solution we found it convenient to integrate over $f$ instead of $\tilde{r}$, similarly to what we did in Sec. 2.1.2 in 1D. This is especially successful for flame models with finite total profile widths. For such models we integrate the following system:

\[
\frac{dn}{df} = \alpha K_0(f)\xi^{-1/\alpha} - \frac{\Phi_0(f)K_0(f)}{n} + d\left(1 + \frac{f}{\Lambda}\right)\left(1 + \frac{I}{\xi}\right) \tag{5.12}
\]
\[
\frac{d\xi}{df} = -\alpha \xi^{-1-1/\alpha}K_0(f) \tag{5.13}
\]
\[
\frac{dI}{df} = \alpha \xi^{-1-1/\alpha}K_0(f)\frac{f}{n} \frac{1}{f + \Lambda}. \tag{5.14}
\]

Here

$\xi = \tilde{r}^\alpha$, $I = \frac{\tilde{r}^\alpha(\tilde{u} - \tilde{u}_0)}{d(H_0 + qf)}$, $n = pK_0(f)$; $p = -\frac{df}{d\tilde{\eta}}$.

$\tilde{u}_0$ is a constant such that $I \to 0$ at $f \to 0$ ($r \to +\infty$). Eq. (5.14) is (5.7) rewritten in terms of $I$, (5.13) is a rewritten definition of $n = -K_0(f) df/d\tilde{\eta}$, and (5.12) is Eq. (5.8) in these new variables.

Boundary conditions at $f = 1$ (left boundary of the flame, $\tilde{r} = \tilde{r}_0$) are

\[
f = 1 : \quad \xi = \tilde{r}_0^\alpha, \quad n = 0. \tag{5.15}
\]

At $f = 0$ (for finite flames this is the right boundary of the flame, located at finite radius $\tilde{r}_0 + w_c$; for flames with an infinite tail into fuel $\tilde{r} = \infty$ at $f = 0$) the boundary conditions are

\[
f = 0 : \quad I = 0, \quad n = 0. \tag{5.16}
\]

This system was integrated from $f = 1$ to $f = 0$. Values of $I_0 = I(f = 1)$ and $d$ were estimated based on 1D results (initial seeding), and then solved for exactly using Newton-Raphson algorithm to satisfy the 2 boundary conditions at $f = 0$.

---

1. We have tried estimating $Ma$ in the approximation of large $\tilde{r}_0$, treating terms $\sim 1/\xi$ with positive powers in Eq. 5.12 as perturbations, using 1D flame profiles $f(\tilde{r})$ in estimating such terms. We only present exact treatment of the problem here for brevity, as approximate consideration is not significantly simpler. Very rough fully analytical estimates may be obtained assuming, say, linear flame profile in perturbation terms; this leads to about 20% error in $Ma$ for finite-width flames.
System (5.12–5.14) is singular at \( f = 1 \) as \( n(1) = 0 \). Because of this integration was actually started at \( 1 - f_\epsilon \) for certain small positive \( f_\epsilon \) (0.01 of bulk integration step); asymptotic expansions for \( \xi, n, I \) were used as initial values at \( f = 1 - f_\epsilon \). For model B (Eq. 3.4) these are

\[
\begin{align*}
n &\equiv pK_0(f) = f_\epsilon^{s_a} + r_a/\phi_0 \\
\xi &= \left( \tilde{r}_0 + \frac{\phi_0}{1 - r_a} f_\epsilon^{1-r_a} \right)^\alpha \\
I &= I_0 - \alpha f_\epsilon^{1-r_a} \frac{\tilde{\rho}_0^{\alpha-1} \phi_0}{(1 - r_a)(1 + \Lambda)}; \\
\phi_0 &\equiv \frac{d}{1 - c(\Lambda)} \left( 1 + \frac{1}{\Lambda} \right) \left( 1 + \frac{I_0}{\tilde{r}_0^\alpha} \right).
\end{align*}
\]

For models A (Eq. 3.1), original model of Khokhlov (1995) (same expression for \( \Phi_0(f), r = 0 \) in the expression for diffusivity \( K \)) and sKPP (3.3) initial asymptotic values used are

\[
\begin{align*}
n &= \nu_0 f_\epsilon^{1/2} \left( 1 + \mu_0 f_\epsilon^{1/2} \right) \\
\xi &= \left[ \tilde{r}_0 + \frac{2}{\nu_0} f_\epsilon^{1/2} \left( 1 - \frac{\mu_0}{2} f_\epsilon^{1/2} \right) \right]^\alpha \\
I &= I_0 - 2 f_\epsilon^{1/2} \frac{\alpha \tilde{\rho}_0^{\alpha-1}}{\nu_0 (1 + \Lambda)} \left[ 1 + \left( \frac{\alpha - 1}{\nu_0 \tilde{r}_0} - \frac{\mu_0}{2} \right) f_\epsilon^{1/2} \right]; \\
\nu_0 &= \sqrt{2\Phi_0(1)} = \left\{ \begin{array}{ll}
\sqrt{2} & \text{for A, Khokhlov (1995)} \\
\sqrt{2\epsilon_a (1 - \epsilon_f)} & \text{for sKPP}
\end{array} \right. \\
\mu_0 &= -\frac{1}{\nu_0} \left[ d \left( 1 + \frac{1}{\Lambda} \right) \left( 1 + \frac{I_0}{\tilde{r}_0^\alpha} \right) + \frac{\alpha}{\tilde{r}_0} \right].
\end{align*}
\]

Resulting curves for \( d(r_0) \) are shown in Fig. 5.1 for Model A, and in Fig. 5.1 for Model B, for 4 expansions each. \( d(r_0)/d(r_0 = \infty) \) is plotted against \( w_1/r_0 \), the slope of the curves at \( w_1/r_0 = 0 \) thus gives Markstein number \( M \). Deviations from linear Markstein law can be seen at larger curvatures. Values of Markstein numbers are shown in Tab. 5.1 in the next section, compared to these numbers estimated in direct numerical simulations.
Figure 5.1: Dependence of flame speed $d$ on curvature, presented in units of inverse flame width $w_1$ for Model A. $d_0 = d(r_0 = \infty)$.

Figure 5.2: Dependence $d(w_1/r_0)$ for Model B.
5.3 Markstein numbers from direct numerical 2D simulations

In this section we estimate how observed numerical flame speed depends on flame curvature, whether one can consistently get Markstein length parameter $Ma$ that would describe this dependence via (5.1) for a range of $r_0$’s as the flame grows in radius. If this is the case, one may further try to correct for this curvature effect on flame speed in multidimensional simulations (by adjusting diffusivity and burning rate parameters based on local flame curvature, so that to correct for the discrepancy in flame speed between plane and curved flames). Comparison between analytical and numerical results clarifies whether real physical Markstein effect dominates unrelated effects (say, growing asphericity of flame surface studied in the previous section leads to apparent growth of $D$ estimated assuming spherical flame shape).

The dependence on $r_0$ we observe deviates from linear form ((5.1) with $Ma_2/R^2$ and further terms in expansion omitted). Contrary to chemical flames, with widths much smaller than radii of curvature studied, our artificial “flame” widths are much wider: $R_0 = 30$ km we typically use as initial flame radius is just about 15 grid cells, and “flame” width $W_1$ is about 4 cells. This difference makes such deviations expectable, after all Markstein “law” is just an expansion over small parameter, which is a ratio of flame width and flame radius of curvature (it is this ratio that determines how strong a stretch on the flame scale is). To make comparisons more consistent we use fits of observed flame speed with (5.1) with 3 terms left in parentheses (that is, (5.1) with “…” omitted), with $Ma, Ma_2$ considered free parameters. We use the same fits to get $Ma, Ma_2$ for $Dr_0$ found analytically. Markstein numbers

$$M = Ma/W_1$$

are reported below (as we saw in Sec. 5.1 analytically, Markstein length $Ma$ scales proportionally to flame width if one changes the latter by varying scale parameters $\tilde{K}, R$ of the model while keeping diffusivity and burning rate form-factors $K_0(f), \Phi_0(f)$ invariant), see Tab. 5.1.

For each model and expansion parameter we present Markstein number $M_{st}$ found analytically, together with that found numerically, for several timesteps and initial setups used. Analytical results shown were obtained by fitting $Dr_0$ found through quasi-steady technique presented in Sec. 5.1–5.2 with 3-term expansion of the form (5.1) for a set of approximately equidistant flame curvatures $1/r_0$, ranging from $1/400$ to $1/50$ (dimensionless, $r_0$ is scaled with the same factor $\sqrt{\tilde{K}/R}$ as dimensionless coordinate $\chi$ and width $w_1$ in Sec. 5.1). As a reminder for the sense of scale, flame width $w_1$ is $\sim 2$ for Model B, and $\sim 8$ for sKPP for small expansion, see Fig. 3.2 and its caption. This way, when fits are used with at least quadratic in curvature terms left in expansion, exact value found for Markstein number $M$ is not sensitive to
precise set of radii used for the fit. Say, if more curvatures are added to cover a range of 0 to 1/15, the $M$ found for Model B at $1/\Lambda = 0.167$ changes from 0.2145 to 0.2117 (1.3%). Besides, when more terms are used in fit (higher powers in curvature left in expansion (5.1)) results for $M$ do not change drastically as well. For the example above leaving terms up to cubic leads to $M = 0.2148$ (for curvature range 0 to 1/15; even smaller difference for reduced range $1/r_0 \in [1/400; 1/50]$, as for $M$’s presented in Tab. 5.1); fit with terms up to quartic in curvature yields $M = 0.2150$.

Numerical Markstein numbers were estimated from 2D runs with central and corner ignition (same setup as in the previous sections). For this, flame speeds and radii were recorded for each timestep; then $D_{R_0}$ was fitted with expansion of the form (5.1) with three terms (up to $r_0^{-2}$) for timesteps from 2000 to the step when flame radius reached the value of $R$ recorded in the column header in Tab. 5.1. Flame speed was estimated based on integral burning rate, $D = -\frac{1}{\rho_{fuel}A}\frac{dm_{fuel}}{dt}$; $A$ here denotes flame surface, estimated based on burned volume assuming spherical flame shape.

| Model         | 1/\Lambda | $M, R_2$ | $M, R_3$ | $M, R_4$ | $M, R_5$ | $M_{st}$ |
|---------------|-----------|----------|----------|----------|----------|----------|
| B             | 0.167     | 0.233    | 0.232    | 0.232    | 0.232    | 0.2145   |
| sKPPq, $N = 512$ | 0.167     | 0.0360   | 0.1506   | 0.1106   | 0.1107   | 0.0733   |
| Bq            | 0.398     | 0.249    | 0.241    | 0.241    | 0.242    | 0.2163   |
| sKPPq         | 0.398     | 0.169    | 0.159    | 0.159    | 0.158    | 0.0680   |
| Bq, $N = 512$ | 0.734     | 0.325    | 0.309    | 0.313    | 0.326    | 0.3246   |
| sKPP          | 0.734     | 0.233    | 0.280    | 0.409    | 0.587    | 0.0588   |
| sKPPq, $N = 512$ | 0.734     | 0.251    | 0.294    | 0.416    | 0.584    | 0.0588   |
| B             | 1.44      | 0.384    | 0.309    | 0.305    | 0.325    | 0.4409   |
| B, $R_0 = 15$ | 1.44      | 0.202    | 0.255    | 0.258    | 0.286    | 0.4409   |
| sKPP          | 1.44      | 0.705    | 2.113    | 3.633    | 6.843    | 0.0517   |
| B, $R_0 = 90$, $N = 2^{11}$ | 2.33     | -        | 0.629    | 1.094    | 2.28     | 0.3432   |
| B, $R_0 = 90$ | 2.33      | -1.69    | 0.760    | 1.134    | 2.48     | 0.3432   |
| B, $R_0 = 90$, $W_1 = 4.5$ | 2.33 | -1.13    | 0.512    | 0.364    | 0.430    | 0.3432   |
| B, $R_0 = 90$, $W_1 = 5$ | 2.33   | -1.64    | 0.517    | 0.325    | 0.339    | 0.3432   |

Table 5.1: Markstein numbers computed numerically for models B and sKPP at timesteps, computed when flame radius reached $R_2 = R_0 + 90$ (km), $R_3 = R_0 + 270$, $R_4 = R_0 + 420$ and $R_5 = R_0 + 600$ (the radius is shown as an index in the table header). Last column shows Markstein number found via quasi-steady state technique.

As follows from the Table, (5.1) consistently describes dependence of flame speed on its radius at small expansions $1/\Lambda$, one gets almost the same Markstein numbers while fitting $D_R$ over different ensembles of $R$’s, meaning that (5.1) is a good approximation, omitted terms are not significant for the curvatures studied. As flame remains circular at these expansions for small enough radii, one would not expect
explicit dependence of flame speed on time, all time dependence is contained in $D_{R(t)}$ dependence, through Markstein effect and radius growth with time. Deviations from this are observed at larger expansions, again expectedly, as corrections to flame speed due to asphericity development (both large-scale, and LD-like) depend explicitly on time provided for the asphericity to develop. For sKPP these deviations are pronounced at $1/\Lambda = 0.734$ and above, in accord with our direct observations of flame distortion development in the previous section. Model B shows similar violation of (5.1) in simulations at $1/\Lambda = 2.33$ ($\rho_{\text{fuel}} = 10^7 \text{ g cm}^{-3}$ in SN Ia problem). This again is in agreement with worse model behavior (faster LD-instability development) at such expansion. Notice that precise $M$ found numerically differs from that found through steady-state technique increasingly as expansion increases. Same increasing deviation was observed above for $D$ in 1D simulations, thus it can be expected that similar discrepancy should be found for curvature corrections to $D$. Increasing flame width damps LD instability development, as well as decreases discrepancy (due to discretization) between numerically found Markstein number, and steady-state one (in continuous calculation). This can be seen in the Table for Model B entries at $1/\Lambda = 2.33$ and different flame width. Notice also, that for $R = R_2$ at $1/\Lambda = 2.33$ one gets negative Markstein numbers. Burning is not quasi-steady yet at that time (timestep 1300) for larger expansions. Studying flame speed as a function of time (what we effectively do through studying Markstein number evolution) provides another way to characterize flame asphericity development.

For smaller expansions agreement with steady-state results for Model B is encouraging. Similar agreement, with further deviation in the same direction due to discretization effects, is observed for 3D simulations; say, we get $M = 0.280$ for Model B $256^3$ cubic run at $1/\Lambda = 0.398$ at $R = R_2 = 120 \text{ km}$ (curvature of a spherical flame in 3D being $2/R$).
We analyzed a reaction-diffusion system (1.3) with hydrodynamically determined advection velocity $u$. This model describes premixed physical flames with one dominating reaction, the rate of which can be effectively determined by one reaction progress variable $f$, which is the case, in part, for systems with unit Lewis number (ideal gases in part); this system is used as a tool for tracking unresolved flames in deflagration simulations (Flame Capturing technique, FC, Khokhlov (1995)), in part in astrophysical simulations of nuclear deflagration in a White Dwarf during an SN Ia explosion.

One part of the study was performed in continuous steady-state approximation (steadily propagating flame solutions) for planar flames (spatially one-dimensional problem; Chap. 1 and 2) with the purpose of finding the flame propagation speed and width, as well as for spherical flames in 2D and 3D, with the goal to quantify Markstein effect, how the flame front speed depends on the its curvature (Chap. 5). For this part of the study we assumed heat release proportional to $f$ increase, $\delta Q = q df$ ($q$ meaning total heat release in the reaction, per unit mass), negligible pressure jump across the flame (thus, in part, thermal enthalpy density increasing linearly with $f$, $dH = \delta Q$, $\rho H = \text{const}$ in the process of such isobaric burning. The problem of finding steady flame profiles $f(x)$ ($f(r)$ for spherical flames) was analytically reduced to finding eigenfunctions of boundary-value problems, (2.10) with $p(0) = p(1) = 0$ for planar flames, (5.12–5.16) for spherical flames. These eigenfunctions yield flame profiles in dimensionless spatial coordinate: all the quantities were made dimensionless by scaling with appropriate powers of characteristic values of reaction rate $R$ and $f$-diffusivity $\tilde{K}$, Eq. (2.7). Dimensionless flame speed $d$, Eq. (2.9) is given by an eigenvalue of the corresponding boundary problem in 1D or nD; for the case of spherical flames flame radius $r_0$ enters explicitly the boundary conditions, thus making flame speed and profile dependent on flame curvature.

Another part of the study was performed numerically, using full hydrodynamical codes ALLA (Khokhlov (1998)) and FLASH (Fryxell et al. (2000)). This part had two major goals. The first one was to check how based on steady analysis calibration of different flame models studied was affected by discretization effects in direct simulations. For flame widths used/proposed to be used in FC (3.2–4 cells between $f = 0.1$ and $f = 0.9$) flame velocities observed in direct simulations are somewhat smaller than their prescribed values based on steady-state analysis, the difference increases with parameter $1/\Lambda$ characterizing matter expansion, Eq. (2.4); this difference remains within 8% for the models studied at $1/\Lambda < 1.44$ (interval of most interest to SN Ia problem, corresponds to fuel (with composition $0.5^{12}C + 0.5^{16}O$) density of $3 \times 10^7 \text{ g cm}^{-3}$ and above). Flame widths observed in these simulations are larger than their prescribed values; Cf. Tab. 2.2 and 3.1 for comparison of continuous and
discretized speeds and widths for some models studied. The discrepancy in width was clearly related to numerical diffusion tails (Fig. 2.9) by increasing number of computation grid cells within the flame width, Tab. 2.3; for such wider flames front speed also tends to its value prescribed through continuous steady-state analysis, discrepancy reduced to about 1% for 16 cells within flame width \( W_1 \).

For thin flames used for FC it is desirable to correct for this discretization discrepancy; this is accomplished by defining dimensionless flame speed \( d \) and width \( w \) by direct simulation in 1D, using flame parameters ensuring physical flame width \( W \) the same as the one to be used for actual simulations (with gravity, arbitrary flame geometry, etc.), see Sec. 3.1.2 for more detail.

For values of \( d \) and \( w \) found by any of the methods (for any flame model, specified by dimensionless form-factors of reaction rate and diffusivity \( \Phi_0 \) and \( K_0 \), (2.7)) the procedure to obtain proper normalization factors \( R \) and \( \tilde{K} \) so that Eq. (1.3) coupled to the rest of hydrodynamic equations yield a “flame” having prescribed width \( W \) and speed \( D \) is given by Eq. (2.37) as described in Sec. 2.5.2. For Model B, in particular, \( d \) and \( w \) are given by fits (A.6), thus yielding efficient procedure for prescribing \( K \) and \( \Phi \) based on local \( \Lambda \).

Any model with unique propagation speed may be calibrated this way to yield a flame with required properties, in idealized conditions at least, in 1D with simple hydrodynamics. Some models are however better than others for use in flame capturing. Certain features of \( \Phi_0 \) and \( K_0 \) of the model used produce flames with undesirable features. Some of these features can be identified in steady state study: for flame models with \( K_0 = 1 \), the original one (Khokhlov (1995), Eq. (2.11)) and KPP (2.12) \( \Phi_0 \) goes to zero either at \( f = 0 \) or 1, thus producing flames with infinite tails. For artificially thickened “flame” used in FC to deviate least in behavior from much thinner physical flame it is imperative to have the flame completely localized in the narrowest possible region. Central region of the “flame”, characterized by large gradients of \( f \) must be adequately resolved in simulations, thus have physical width of about 3 or more grid spacings; therefore flames without long tails, with profile close to linear are to be preferred. By small perturbation of the burning rate model KPP may be transformed into a model with finite tails (and unique eigenvalue for propagation speed), sKPP, Eq. (3.3). However unless the perturbation (given by shift parameters \( \epsilon_a, \epsilon_f \)) is large enough (leading to significant numerical noises) model sKPP retains long tails in the profile (Fig. 3.4), thus having a disadvantage compared to other models proposed.

Using non-constant diffusivity, \( K_0 = f^r \) allows one to make a model with step-function burning rate have finite tails; choice of parameters \((f_0; r) = (0.2; 0.75)\) makes flame profiles insensitive to flame expansion, another desirable feature to make “flame” response to hydrodynamics similar at different densities (in SN Ia problem), consistent throughout the simulation as the flame propagates into less dense regions further from the center of the WD. However this model, Model A, as well as other
models with large discontinuities in burning rate produces significant numerical noises in simulations, about 10% fluctuations in instant flame speed, Fig. 3.5. Numerical noises, as well as flame propagation anisotropy, small-scale hydrodynamical instability of the flame front in 2D and 3D are only observed in actual simulations of discretized on computation grid set of hydrodynamic equations, not in continuous steady-state study. Studying these intrinsically non-steady features of the flames was another major goal of numerical part of our study, presented mostly in Chap. 3 and 4.

Numerical study showed that different models differ one from another in amount of noise they produce (which is readily observed in 1D), in flame surface distortion in 2D and 3D. 1D noises and flame speed anisotropy with respect to the grid are numerical artifacts and must be minimized by choosing appropriate flame model for use in FC. Small scale instability we observed on spherical, cylindrical and perturbed planar flames is of physical nature, characteristic for any flame propagation when fuel and ash densities differ. This instability is of the type studied by Landau and Darrieus in simplified setting, as was demonstrated by quantitative agreement between characteristic instability lengthscales in our direct simulations, and analytic estimates in Markstein approximation, Sec. 4.4. It is physically impossible to invent a flame model immune to this instability. However some models, like sKPP, become fast perturbed on very small scales, of order 10 cells at $1/\Lambda \geq 0.734$, whereas another model proposed, Model B, Eq. (3.4–3.7), only starts showing signs of this instability development (at $1/\Lambda \geq 1.44$) when getting close to boundaries in $1024 \times 1024$ box, in cylindrical flame simulations; flame radius increasing by a factor of 20 by that time, Fig. 4.1. Such behavior is adequate for SN Ia simulations. Numerical effects, propagation anisotropy and noises, are also insignificant for Model B, whereas sKPP shows significant anisotropy at $1/\Lambda \gtrsim 0.734$, which strongly distorts the pattern of LD-type instability.

Flames of Model B are not perturbed significantly by reflecting boundaries, in contrast with sKPP, for which octant simulations are thus even more questionable. Markstein numbers computed for Model B using quasi-steady state technique, Sec. 4.4.1 and estimated based on radius dependence of cylindrical flame speed $D(r_0)$ in simulations demonstrate close agreement at small expansions, and are close enough at $1/\Lambda = 1.44$ to suggest that physical Markstein effect dominates over contribution to $D(r_0)$ dependence due to propagation anisotropy and LD-instability at densities of $\gtrsim 3 \times 10^7$ g cm$^{-3}$ in WD problem. Based on all these features observed we recommend using Model B for Flame Capturing.

A few directions to develop that are close to our study are the following.

- Larger 3D simulations need to be performed to clearly see LD-instability on spherical flames for Model B. The results might suggest slight changes in the model, better behavior in 3D may be possible with somewhat larger $c(\Lambda)$ term in burning rate at large expansions.
To use the model when $H\rho$ is significantly nonconstant (which is the case in SN Ia problem at smaller densities, $\sim 10^6 g cm^{-3}$, near quenching of nuclear burning) steady-state model calibration has to be modified; this is automatically corrected for if the model is calibrated numerically, as is the case for Model B calibration (A.6).

Also at smaller densities in SN Ia problem assumptions of the flame being isobaric becomes increasingly violated. This is due to decreasing sound speed, and increasing speed of the flame with respect to the grid, equal to $D(1 + 1/\Lambda)$ for planar flames. As follows from analysis in Sec. 2.1.1 flame speed depends on exact density distribution within the flame in part, which is affected by pressure jump across the flame and should be corrected for if this jump is significant. The jump depends on geometry of the flow: in our simulations this non-isobaricity led to systematic increase of flame speed in 2D and 3D as compared to the speed in 1D. The deviation reached 1% at $1/\Lambda = 2.33$, and $\sim 20\%$ at $1/\Lambda = 8.57$ (at that density, $8 \times 10^5 g cm^{-3}$, sound speed is just a factor of 2 larger than $D(1 + 1/\Lambda)$, for $D = 80 km s^{-1}$ used.) These problems of equation of state and large pressure jump should not be relevant for most terrestrial flames.

Quasi-steady state technique presented in Sec. 5.1 in general setting, with arbitrary Lewis number and possibility of having several species involved in reactions with comparable rates is immediately applicable for quasi-steady estimates of Markstein widths of various terrestrial and astrophysical problems. The same technique, simplified to planar flames, may be used to find steady propagation velocities of flames more general than the ones described by Eq. (1.3). This may be needed even for some FC models that involve more than one reaction progress variable, with intent to more accurately prescribe heat release distribution when several characteristic reactions with different enough characteristic temporal and spacial scales are to be taken into account.
APPENDIX A
SUMMARY OF IMPLEMENTATION OF FC TECHNIQUE WITH FLAME MODEL B

Here we summarize a step-by-step instructions for using the Flame Capturing Technique based on Model B we recommend based on analysis in the thesis.

Assuming one has a hydrodynamic solver for modeling deflagrations, the steps to use the technique for tracking the thickened flame region are the following:

1) Add one new scalar quantity $f$ to physical variables evolved with the code.

2) Use $\delta Q/dt = q df/dt$ as a heat release term in original hydrodynamic equations. $q$ is total specific heat release of nuclear burning, it depends on local pressure and fuel composition.

3) Evolve $f$ via

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f = \nabla (K \nabla f) + \Phi(f), \quad (A.1)$$

where $\mathbf{u}$ stands for local gas velocity, source term and diffusivity are given by

$$\Phi(f) = R f^s f (1 - f)^s_a (f - c(\Lambda)), \quad (A.2)$$

$$K(f) = \tilde{K} f^r f (1 - f)^r_a. \quad (A.3)$$

respectively,

$$s_f = 1, \ s_a = 0.8, \ r_f = 1.2, \ r_a = 0.8. \quad (A.4)$$

Normalization factors $\tilde{K}$ and $R$ are functions of locally determined expansion parameter $\Lambda = \rho_{ash}/(\rho_{fuel} - \rho_{ash})$ (the latter depends on pressure and fuel composition in the cell), and the values for “flame” speed $D$ and width $W_1$ (between values $f = 0.1$ and $f = 0.9$) one strives to obtain:

$$\tilde{K} = \frac{D_f}{d(\Lambda)} \frac{W_1}{w_1(\Lambda)}, \quad R = \frac{D_f}{d(\Lambda)} \big/ \frac{W_1}{w_1(\Lambda)}. \quad (A.5)$$
Dimensionless \( d(\Lambda) \), \( w(\Lambda) \), and term \( c(\Lambda) \) in Eq. (A.2) are given by the following fits:

\[
\begin{align*}
1/\Lambda & \in [0; 0.515] : \\
& \begin{cases} 
  c = 0.005 \\
  d = 0.328227 - 0.10051/\Lambda + 0.0244596/\Lambda^2 \\
  w_1 = 2.075422 + 0.443918/\Lambda - 0.097483/\Lambda^2 \\
  c = 1/\Lambda - 0.51 \\
  d = 0.497578 - 0.363476/\Lambda + 0.1036/\Lambda^2 \\
  w_1 = 1.553031 + 1.50381/\Lambda - 0.192923/\Lambda^2 \\
  c = 0.3 \\
  d = 0.172133 - 0.051673/\Lambda + 0.0073512/\Lambda^2 \\
  w_1 = 2.475085 + 0.232926/\Lambda - 0.0323989/\Lambda^2 \\
  c = 0.675 - 0.25/\Lambda \\
  d = -0.0420695 + 0.129058/\Lambda - 0.0177843/\Lambda^2 \\
  w_1 = 2.764056 - 0.0061156/\Lambda + 0.0025170/\Lambda^2 \\
  c = 0.2 \\
  d = 0.0139649 + 0.434752\Lambda - 0.507838\Lambda^2 + 0.250103\Lambda^3 \\
  w_1 = 3.3891706 - 2.857323\Lambda + 5.045909\Lambda^2 - 3.744233\Lambda^3.
\end{cases}
\end{align*}
\]

These fits yield errors in flame speed in 1D not exceeding 0.8% for \( W_1 = 3.2 \) cells, the value we recommend to use, and \( 1/\Lambda \in [0; 8.6] \), covering expansions of interest for SN Ia problem.
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