Software Impacts 15 (2023) 100480

Contents lists available at ScienceDirect

Software Impacts

journal homepage: www.journals.elsevier.com/software-impacts

Original software publication

# PaSR-SDE: Premixed turbulent combustion with stochastic mixing models simulator

Elder Mendoza Orbegoso [a], Luís Fernando Figueira da Silva [b,c], Americo Cunha Jr [d,*]

[a] Universidad Nacional de Trujillo, Peru
[b] Institut Pprime, UPR 3346 CNRS, ENSMA and Université de Poitiers, France
[c] Pontifícia Universidade Católica do Rio de Janeiro, Brazil
[d] Universidade do Estado do Rio de Janeiro, Rio de Janeiro, Brazil

## ARTICLE INFO

*Keywords:*
Partially stirred reactor
Probability Density Function
Premixed turbulent combustion
Mixing models
Stochastic Differential Equation
Monte Carlo simulation

## ABSTRACT

Approaches based on Probability Density Function Differential Equation (PDF-DE) have been used for modeling premixed turbulent combustion under Eulerian frame reference, but their solution requires the diffusion phenomena to be closed. In this context, Stochastic Differential Equations (SDEs) are an alternative method to solve the PDF-DE under a Lagrangian reference. **PaSR-SDE** is a Matlab package that solves the Partially Stirred Reactor mathematical formulation that takes into account mixing models for the closure of the term describing the scalar diffusion, and it is also used as a numerical tool in evaluating the influence of several mixing models on the thermochemical properties in a premixed turbulent combustion situation.

## Code metadata

| | |
|---|---|
| Current code version | 2.0 |
| Permanent link to code/repository used for this code version | https://github.com/SoftwareImpacts/SIMPAC-2023-48 |
| Permanent link to Reproducible Capsule | https://codeocean.com/capsule/3034874/tree/v1 |
| Legal Code License | MIT |
| Code versioning system used | Git |
| Software code languages, tools, and services used | Matlab |
| Compilation requirements, operating environments & dependencies | |
| If available Link to developer documentation/manual | https://github.com/americocunhajr/PaSR-SDE |
| Support email for questions | eldermendoza@gmail.com |

## 1. Introduction

Among the recent challenges in studying turbulent reactive flows is the development of computational models capable of adequately describing the interactions between combustion, turbulence, and mixing of reactants [1–4]. The Partially Stirred Reactor (PaSR) approach can take into account the coupling between a detailed description of the chemical process and the micro-mixing process between reactants and combustion gases, i.e., the presence of fluctuations in thermodynamic properties during combustion, which is directly related to the influence of the degree of mixing during its process, which can lead to a higher rate of pollutant formation.

The mathematical formulation of PaSR can be accomplished by using the transport equation of a Probability Density Function (PDF) [3–5]. When models that consider the PDF transport of flow properties are used, the convection and chemical production terms appear closed-ended and therefore do not require modeling. However, the scalar field diffusion or micromixing phenomenon remains open-ended and therefore needs modeling [6–13]. This difficulty arises because diffusive processes involve two-point type formulations, which statistical techniques of the one-point type cannot describe.

The code (and data) in this article has been certified as Reproducible by Code Ocean: (https://codeocean.com/). More information on the Reproducibility Badge Initiative is available at https://www.elsevier.com/physical-sciences-and-engineering/computer-science/journals.

* Corresponding author.
*E-mail addresses:* eldermendoza@unitru.edu.pe (E.M. Orbegoso), luis-fernando.figueira-da-silva@ensma.fr (L.F. Figueira da Silva), americo.cunha@uerj.br (A. Cunha Jr).

https://doi.org/10.1016/j.simpa.2023.100480
Received 30 January 2023; Received in revised form 9 February 2023; Accepted 13 February 2023

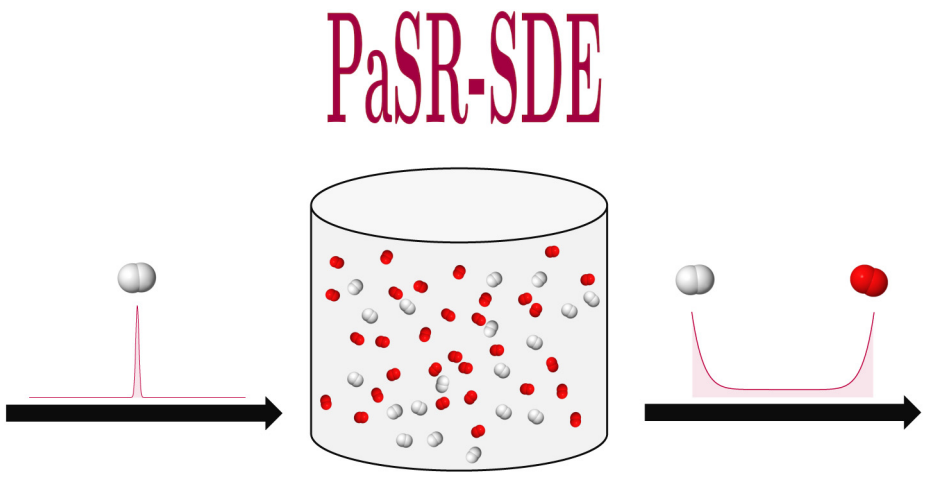


**Fig. 1.** **PaSR-SDE** is a tool to simulate premixed turbulent combustion in a PaSR reactor.

In the past decades, several models have been proposed to represent the micro-mixture process, starting with the interaction through Interaction by Exchange with the Mean model [14], up to more sophisticated ones, such as the Langevin models [5,15]. Sabel'nikov and Gorokhovski [16] proposed stochastic mixing models, the most complex and functional, the Extended Interaction by Exchange with the Mean model (EIEM) and the Extended Langevin Model (ELM). Both models replace the single time scale used in the IEM and Langevin models with a stochastic description of the frequency of turbulent motion and by adding a term that simulates the dissipation of the scalar field, which leads to a scattering of the phase space trajectories while ensuring the boundedness property. Therefore, it is possible to achieve a PDF relaxation from an inert scalar field to a Gaussian shape of a single transported scalar.

Despite the significant increase in open-source codes for the simulation of reactive processes seen in the last decade, mainly driven by developers and users of Open FOAM [17], and Cantera [18] packages, the literature is still lacking in Matlab codes to simulate chemical processes with stochastic micro-mixing models. Seeking to fulfill this gap and expand the arsenal of open-source tools to simulate premixed turbulent combustion in a PaSR reactor, this paper introduces a Matlab package named **PaSR-SDE** (Fig. 1).

## 2. Software details

The **PaSR-SDE** package is a Matlab code that solves the governing equations of a PaSR considering for model closure one of the following micro-mixing models: IEM, EIEM, LM, and ELM. In this setting, the outcome of the combustion process is governed by the competition between the characteristic time scales of the chemical reaction, mixing, and the residence time of the gases inside the PaSR. The PDF transport equation is solved employing an equivalent system of stochastic differential equations (SDEs) using the Monte Carlo technique [19,20], using the [21] implicit numerical method. This allows obtaining a characterization of the transported scalar in terms of statistical properties like mean, variance, kurtosis, or other high-order moments.

The code has a modular structure, and each routine/function has a detailed description of its functionality via internal comments. Version 2.0 is compatible with Matlab 2016a or newer. Extensions of the code are relatively simple to implement due to its modular structure so that it can be easily coupled with existing libraries for combustion simulation like Cantera [18] or CRFlowLib [22].

## 3. Impact overview

**PaSR-SDE** was developed at the *Pontifícia Universidade Católica do Rio de Janeiro (PUC-Rio)*, between 2005 and 2007, during the first author's master course [8], under the supervision of the second author. The results of this dissertation, obtained with the code, were published in the Proceedings of the Combustion Institute [9]. Over the years, the first version of the code became incompatible with newer versions of Matlab, requiring a review, reformulation, and updating of practically all code modules. Such changes were introduced in early 2023 by the third author, who introduced detailed comments in English in all the code modules, seeking to provide the end user with an accessible tool.

The open-source movement has sparked a trend toward creating code that is not only functional but also educational [23–31]. **PaSR-SDE** follows this trend, offering the following features:

- Real-world applications: Simulating premixed turbulent combustion in a partially stirred reactor is a relevant and practical problem in energy and combustion engineering. By using PaSR-SDE, students can learn how to model and analyze real-world problems, which is a valuable skill in engineering and science;
- Understanding of SDEs: Stochastic differential equations are widely used in engineering, physics, and finance. By using **PaSR-SDE**, students can see how an SDE solver is implemented, which is a fundamental skill for experts in these areas;
- Hands-on experience with simulation: Once it is a Matlab code, **PaSR-SDE** provides a user-friendly interface for simulating premixed turbulent combustion, which is a complex process. By using the code, students can gain hands-on experience with simulation, which is a valuable skill in engineering and science;
- Understanding of combustion dynamics: The simulation of premixed turbulent combustion involves the interplay between fluid mechanics, heat transfer, and chemical reactions. By using **PaSR-SDE**, students can better understand these processes, which is essential for solving real-world problems in the energy and combustion engineering field.

In comparison to other open-source codes that simulate the dynamics of a partially stirred reactor, such as CRFlowLib (C/C++) [22], ISAT-CK7 (Fortran) [32], and PyJac (Python) [33], **PaSR-SDE** sets itself apart by incorporating more advanced micro-mixing models such as EIEM and ELM. The authors believe that this decision brings two pedagogical benefits to the table when using **PaSR-SDE** as an educational tool: (i) providing students with a simulator that has more realistic

physical chemistry, and (ii) allowing students to engage with stochastic differential equations as a modeling tool, which is not typically taught in standard numerical methods courses. Despite the computational efficiency offered by CRFlowLib and ISAT-CK7, implemented in low-level languages, **PaSR-SDE** stands out for its ease of use, as the Matlab environment is usually more accessible for beginner students compared to C/C++ or Fortran.

In conclusion, **PaSR-SDE** is an open-source research and educational tool that has the potential to be of great utility for the academic and industrial community working with the simulation of reactive processes.

## 4. Final remarks

**PaSR-SDE** is a computational package that provides an extensive framework to analyze an ideal partially stirred reactor with several types of micro-mixing stochastic models. Due to its modular structure, the code can be used together with other codes/libraries to simulate combustion systems (e.g., CRFlowLib [22]). Once very few open-source packages exist to simulate combustion systems stochastic micro-mixing models, this package may be a helpful research and educational tool that can contribute to the community of reactive flow simulation.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Acknowledgments

The authors are indebted to the Brazilian agencies National Council for Scientific and Technological Development (CNPq), Coordination for the Improvement of Higher Education Personnel (CAPES), and Research Support Foundation of the State of Rio de Janeiro (FAPERJ) for the financial support given to this research. During this work L. F. Figueira da Silva was on leave from Intitute Pprime, Centre National de la Recherche Scientifique (CNRS).

## Disclaimer

This manuscript underwent a thorough grammatical revision and improvement with the assistance of artificial intelligence-powered tools such as Grammarly and ChatGPT. Nevertheless, the authors retain full responsibility for the original language and phrasing.

## References

[1] A.L.D. Bortoli, G.S.L. Andreis, F.N. Pereira, Modeling and Simulation of Reactive Flows, Elsevier, 2015.
[2] C. Celis, L.F. Figueira da Silva, Lagrangian mixing models for turbulent combustion: Review and prospects, Flow Turbul. Combust. 94 (2015) 643–689, http://dx.doi.org/10.1007/s10494-015-9597-1.
[3] R.O. Fox, Computational Models for Turbulent Reacting Flows, Cambridge University Press, 2003.
[4] S.B. Pope, Turbulent Flows, Cambridge University Press, 2000.
[5] S.B. Pope, PDF methods for turbulent reactive flows, Prog. Energy Combust. Sci. 11 (1985) 119–192, http://dx.doi.org/10.1016/0360-1285(85)90002-4.
[6] V.A. Sabel'nikov, L.F. Figueira da Silva, Partially stirred reactor: Study of the sensitivity of the Monte-Carlo simulation to the number of stochastic particles with the use of a semi-analytic, steady-state, solution to the PDF equation, Combust. Flame 129 (1) (2002) 164–178, http://dx.doi.org/10.1016/S0010-2180(02)00336-X.
[7] O. Soulard, V. Sabel'nikov, M. Gorokhovski, Stochastic scalar mixing models accounting for turbulent frequency multiscale fluctuations, Int. J. Heat Fluid Flow 25 (2004) 875–883, http://dx.doi.org/10.1016/j.ijheatfluidflow.2004.03.008.
[8] E.M.M. Orbegoso, Estudo De Modelos De Mistura Estocáasticos Para a Combustãao Em Escoamentos Turbulentos (Master Dissertation), Pontifícia Universidade Católica do Rio de Janeiro, Rio de Janeiro, 2007, (in Portuguese).
[9] E.M. Orbegoso, L.F. Figueira da Silva, Study of stochastic mixing models for combustion in turbulent flows, Proc. Combust. Inst. 32 (2009) 1595–1603, http://dx.doi.org/10.1016/j.proci.2008.06.008.
[10] F.O. Andrade, L.F. Figueira da Silva, A. Mura, Large eddy simulation of turbulent premixed combustion at moderate Damköhler numbers stabilized in a high-speed flow, Combust. Sci. Technol. 183 (7) (2011) 645–664, http://dx.doi.org/10.1080/00102202.2010.536600.
[11] A. Cunha Jr., L.F. Figueira da Silva, Assessment of a transient homogeneous reactor through in situ adaptive tabulation, J. Braz. Soc. Mech. Sci. Eng. 36 (2) (2014) 377–391, http://dx.doi.org/10.1007/s40430-013-0080-4.
[12] C. Celis, L.F. Figueira da Silva, Study of mass consistency LES/FDF techniques for chemically reacting flows, Combust. Theory Model. 19 (4) (2015) 465–494, http://dx.doi.org/10.1080/13647830.2015.1048828.
[13] C. Celis, L.F. Figueira da Silva, On the non-equilibrium behavior of fuel-rich hydrocarbon/air combustion within perfectly stirred reactors, Combust. Sci. Technol. 189 (2017) 732–746, http://dx.doi.org/10.1080/00102202.2016.1248239.
[14] J. Villermaux, J. Devillon, Représentation de la Redistribution des Domaines de Ségrégation dans un Fluide par um Modèle D'interaction Phénomenologique, in: 2nd International Symposium of Chemical Reacting Engineering, Amsterdam, Netherlands, 1972.
[15] L. Valiño, C. Dopazo, A binomial Langevin model for turbulent mixing, Phys. Fluids A 3 (12) (1991) 3034–3037, http://dx.doi.org/10.1063/1.857847.
[16] V. Sabel'nikov, M. Gorokhovski, Extended LMSE and langevin models of the scalar mixing in turbulent flows, in: Second International Symposium of Turbulence an Shear Flow Phenomena, Royal Institute of Technology (KTH), Stockholm, Sweden, 2001.
[17] Open FOAM, 2021, www.openfoam.com.
[18] D.G. Goodwin, H.K. Moffat, I. Schoegl, R.L. Speth, B.W. Weber, Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes, 2022, http://dx.doi.org/10.5281/zenodo.6387882, Version 2.6.0, https://www.cantera.org.
[19] C. Gardiner, Stochastic Methods: A Handbook for the Natural and Social Sciences, Springer-Verlag Berlin Heidelberg, 2009.
[20] D.P. Kroese, T. Taimre, Z.I. Botev, Handbook of Monte Carlo Methods, Wiley, 2011.
[21] T. Tian, K. Burrage, Implicit Taylor methods for stiff stochastic differential equations, Appl. Numer. Math. 38 (2001) 167–185, http://dx.doi.org/10.1016/S0168-9274(01)00034-4.
[22] A. Cunha Jr., L.F. Figueira da Silva, CRFlowLib – Chemically Reacting Flow Library, Softw. Impacts 11 (2022) 100206, http://dx.doi.org/10.1016/j.simpa.2021.100206.
[23] J.P. Norenberg, J.V. Peterson, V.G. Lopes, R. Luo, L. de la Roca, M. Pereira, J.G.T. Ribeiro, A. Cunha Jr, STONEHENGE – Suite for nonlinear analysis of energy harvesting systems, Softw. Impacts 10 (2021) 100161, http://dx.doi.org/10.1016/j.simpa.2021.100161.
[24] A.A. Brum, G.C. Duarte-Filho, R. Ospina, F.A.G. Almeida, A.M.S. Macêdo, G.L. Vasconcelos, ModInterv: An automated online software for modeling epidemics, Softw. Impacts 14 (2022) 100409, http://dx.doi.org/10.1016/j.simpa.2022.100409.
[25] A. Cunha Jr., F.d.C. Batista, P.R.d.L. Gianfelice, R.S. Oyarzabal, J.M.V. Grzybowski, E.E.N. Macau, epidWaves: A code for fitting multi-wave epidemic models, Softw. Impacts 14 (2022) 100391, http://dx.doi.org/10.1016/j.simpa.2022.100391.
[26] M. Tosin, E. Dantas, A. Cunha Jr., R.E. Morrison, ARBO: Arbovirus modeling and uncertainty quantification toolbox, Softw. Impacts 12 (2022) 100252, http://dx.doi.org/10.1016/j.simpa.2022.100252.
[27] B. Pavlack, M. Grave, E. Dantas, J. Basilio, L. de la Roca, J. Norenberg, M. Tosin, L. Chaves, D. Matos, M. Issa, R. Luo, A. Guyt, L. Soares, R. Burgos, L. Lovisolo, A. Cunha, EPIDEMIC - Epidemiology educational code, J. Open Source Educ. 5 (2022) 149, http://dx.doi.org/10.21105/jose.00149.
[28] M. Tosin, A.M.A. Cortes, A. Cunha Jr, A tutorial on Sobol' global sensitivity analysis applied to biological models, in: F. da Silva, N. Carels, M. Trindade dos Santos, F. Lopes (Eds.), Networks in Systems Biology: Applications for Disease Modeling, Springer International Publishing, Cham, 2020, pp. 93–118, http://dx.doi.org/10.1007/978-3-030-51862-2_6.
[29] FEniCS, 2023, www.fenicsproject.org.
[30] C. Talischi, G.H. Paulino, A. Pereira, I.F. Menezes, PolyMesher: A general-purpose mesh generator for polygonal elements written in Matlab, Struct. Multidiscip. Optim. 45 (2012) 309–328, http://dx.doi.org/10.1007/s00158-011-0706-z.
[31] C. Talischi, G.H. Paulino, A. Pereira, I.F.M. Menezes, PolyTop: A Matlab implementation of a general topology optimization framework using unstructured polygonal finite element meshes, Struct. Multidiscip. Optim. 45 (2012) 329–357, http://dx.doi.org/10.1007/s00158-011-0696-x.
[32] S. Pope, V. Hiremath, S. Lantz, Z. Ren, L. Lu, ISAT-CK7: A Fortran 90 library to accelerate the implementation of combustion chemistry, 2012, http://tcg.mae.cornell.edu/ISATCK7.
[33] K.E. Niemeyer, N.J. Curtis, pyJac v1.0.6, 2018, http://dx.doi.org/10.5281/zenodo.1182789, URL https://github.com/slackha/pyJac.