Tools for Design and Scale-Up of Solar Thermochemical Reactors

Cooperative Research and Development Final Report

CRADA Number: CRD-13-00530

NREL Technical Contact: Ray Grout

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Technical Report
NREL/TP-2C00-83353
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NOTICE

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Cooperative Research and Development Final Report

Report Date: June 29, 2022

In accordance with requirements set forth in the terms of the CRADA agreement, this document is the CRADA final report, including a list of subject inventions, to be forwarded to the DOE Office of Scientific and Technical Information as part of the commitment to the public to demonstrate results of federally funded research.

Parties to the Agreement: University of New South Wales

CRADA Number: CRD-13-00530

CRADA Title: Tools for Design and Scale-Up of Solar Thermochemical Reactors

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Sponsoring DOE Program Office(s):

- U.S. Department of Energy Office of Science (SC), Advanced Scientific Computing Research (ASCR)
- NREL Facilities and Infrastructure Program

Joint Work Statement Funding Table showing DOE commitment:

Estimated Costs	NREL Shared Resources a/k/a Government In-Kind
Year 1	$315,774.00
Year 2	$315,774.00
Year 3	$315,774.00
Year 4, Modification #1	$0.00
Year 5, Modification #2	$0.00
Year 6, Modification #3	$0.00
Year 7, Modification #4 & 5	$0.00
TOTALS	$947,322.00

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Executive Summary of CRADA Work:

NREL will be collaborating with the Participant on a United States – Australia Solar Energy Collaboration (USASEC) Project Number 1-USO034 "Tools for design and scale-up of solar thermochemical reactors". The grant funds for the Participant's 3.5 year project number 1-US034 commencing on 1 February 2013 have been awarded to the Participant by the Australian Renewable Energy Agency and NREL will be collaborating with the Participant during the final 28 months of this project. This project seeks to provide basic knowledge required to design solar thermochemical reactors able to perform the required energy conversions. In several proposed and demonstrated reactors, concentrated sunlight directly irradiates small solid particles suspended in fluid, enabling very high heat transfer rates to the particles which are the sites of chemical reaction. The reactors, therefore, involve the complex and couple dynamics of turbulent, chemically reacting, particle-laden flows and their interaction with concentrating solar radiation. A strong understanding of these coupled interactions will be crucial important in predicting and optimizing the performance of prototype reactors, but this understanding does not yet exist, since they have never been studied in any fundamental way.

The project has assembled an internationally leading team from The University of New South Wales (UNSW) and the University of Adelaide in Australia and the NREL in the United States to address this key gap in available know-how. The project will use U.S. Dept. of Energy (DOE) supercomputers, among the most powerful available worldwide, with cutting-edge software tools to perform first-principles simulations of the relevant interactions. These studies will be combined with detailed laser-based measurements in Australia to provide the first comprehensive databases concerning the governing phenomena in directly irradiated solar-thermochemical reactors. The outcomes will be the basic scientific knowledge, engineering knowhow and modeling tools necessary to design new reactor concepts and then scale up from the laboratory bench to practical size systems.

CRADA benefit to DOE, Participant, and US Taxpayer:

University of New South Wales will contribute expertise and advice on the coupling between reacting particles and a reacting gas phase flow and "performance analysis on prototype implementations" enabling the solar energy project to make effective use of computational resources and codesign to gather feedback on the usefulness of the work we have been doing and NREL. The plan is to make a miniapp derived from the implementation that UNSW puts together out of this project for use in United States.

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Summary of Research Results:

NREL and UNSW collaborated to perform direct numerical simulation (DNS) of thermochemical particles in a turbulent flow. These simulations generated datasets that were validated against experimental measurements and, as part of the broader ARENA Project 1-USO-034, used to develop the fundamental understanding and models necessary for engineering design simulations of solar thermochemical receivers. The collaboration is comprised of two work packages: (1) extension of an existing DNS code to account for heating of the particles by the absorption of solar radiation in a formulation suitable for running on NREL's supercomputing facilities and (2) carrying out of the simulations to provide the necessary datasets for the balance of the project.

Task 1: NREL will provide expertise and advance on the coupling between reacting particles and a reacting gas phase flow; performance analysis of the prototype implementations of the irradiation physics on NREL's supercomputers; host UNSW; provide computing resources for code development and testing. UNSW with collaborate with NREL on the algorithmic design and support the labor necessary to implement the algorithms in the computational code.

This project developed two new capabilities necessary for high fidelity simulation of solar thermochemical systems to an existing DNS tool long developed with DOE support and significant input from the PIs at NREL and Participant (Ray Grout and Evatt Hawkes). The two new capabilities include: i) models to enable simulation of a poly- disperse discrete solid phase, and ii) models to enable simulation of solar radiation heat transfer. This builds on a strong collaboration between two internationally leading groups using DNS–UNSW and NREL–to move from gas phase combustion to particle-laden flows with chemical reaction and radiation transport. DNS is a fine-grained, first-principles approach that requires supercomputing resources to apply. It is used to understand such flows at a fundamental level, and to validate less detailed engineering models of the flows which are applicable in engineering design and do not require supercomputers to run. In the project, we successfully developed the first DNS tool capable of simulating the coupled phenomena of turbulence, radiation, particles and chemistry [1, 2].

For the first capability, NREL hosted two visiting scholars from UNSW during which time several design decisions, algorithmic design and code develop was done collaboratively. In DNS, the gas phase equations are solved without any models for turbulent motion; in the treatment used here the particles were approximated using a point-particle approach. The gas phase equations are modified to include particle interaction through a feedback force to the flow that is added to the momentum equation:

$$\frac{\partial(\rho u_i)}{\partial t}+\frac{\partial}{\partial x_j}\left(\rho u_i u_j\right)=\frac{\partial \sigma_{ij}}{\partial x_j}+F_i \qquad \sigma_{ij}=-P\delta_{ij}+\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}-\frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right)$$

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Where ρ is the density, u_i is the i^{th} component of the flow velocity **u**, P is the pressure**,** μ is the dynamic viscosity of the flow, and δ_{ij} is the Kronecker delta. **F** represents the feedback force to the flow by the particles and F_i is the i^{th} component of **F** The remaining conservation equations that describe reacting multi-component gas phase conservation (the Navier-Stokes system) are unchanged. Particles are modeled with a point-particle approach which has been shown to be reasonable in DNS where the particle size is much smaller than the smallest turbulence length scale and the particle volume fraction is small [3]. The particles are evolved in time using a Lagrangian framework where the trajectory of the particles is computed by explicitly integrating the equation of motion with contributions to the total force from, in this case, Stokes drag as the dominating force [4,5] and Saffman lift to capture the effect of large velocity gradients [6], that is:

$$m_p \frac{d\mathbf{v}}{dt} = \mathbf{F}_D + \mathbf{F}_s$$

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}$$

Where the drag force given by [7]:

$$\mathbf{F}_D = \frac{1}{2}\frac{\rho\pi d_p^2}{4} C_D(\mathbf{u}(\mathbf{x},t)-\mathbf{v})\,|\,\mathbf{u}(\mathbf{x},t)-\mathbf{v}\,| \qquad C_D = \frac{24}{\mathrm{Re}_p}(1+0.15\,\mathrm{Re}_p^{0.687})$$

And the Saffman lift due to shear is [6]:

$$\mathbf{F}_s = \frac{\rho}{2}\frac{\pi d_p^3}{4} C_L((\mathbf{u}(\mathbf{x},t)-\mathbf{v})\times\boldsymbol{\omega})$$

$$C_L = \frac{4.1126}{\mathrm{Re}_s} f(\mathrm{Re}'_P, \mathrm{Re}_s)$$

$$f(\mathrm{Re}'_P, \mathrm{Re}_s) = \begin{cases} (1-0.3314\beta^{0.5})e^{-(\mathrm{Re}'_P/10)} + 0.3314\beta^{0.5} & \mathrm{Re}'_P \le 40 \\ 0.0524(\beta\,\mathrm{Re}'_P)^{0.5} & \mathrm{Re}'_P > 40 \end{cases}$$

$$\beta = \mathrm{Re}_s/(2\,\mathrm{Re}'_P)\,,\ \mathrm{Re}'_P = d_p\,|\,\boldsymbol{\omega}\,|/(2\,|\,\mathbf{u}(\mathbf{x},t)-\mathbf{v}\,|)\,,\ \mathrm{Re}_s = d_p^2\,|\,\boldsymbol{\omega}\,|/\nu\,.$$

During the two visits, UNSW implemented the above equations into the S3D codebase and conducted performance analysis and tuning under the guidance of NREL.

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For the second capability—models to enable simulation of solar radiation heat transfer—the project developed two formulations: a discrete ordinates method [8] and a photon Monte Carlo (PMC) approach. The NREL effort centered on an implementation and performance optimization of the PMC approach described by Modest [9] that could be coupled to the S3D DNS code. Ultimately, the project elected to pursue the discrete ordinates method for later simulations given the overall computational cost of the PMC approach, but the PMC capability was released as open source software [10,11] so that it is available for future use by this or other project teams.

The PMC approach is designed to solve the radiative transfer equation that depends on space, time, wavenumber and direction:

$$\frac{dI_\eta}{ds} = k_\eta I_{b\eta} - k_\eta I_\eta - \sigma_{s\eta} I_\eta + \frac{\sigma_{s\eta}}{4\pi} \int_{4\pi} I_\eta(\hat{s}_i)\Phi_\eta(\hat{s}_i, \hat{s})d\Sigma,$$

,

Where the terms represent the change of intensity in the direction s due to emission, absorption, scattering away from s and scattering into direction s from other directions. Wang and Modest [8] solve this equation with the aid of a discrete particle method where the medium is represented by a collection of virtual particles representing the medium. Grout [10] modified the method slightly to represent a physical particle field with a non-participating intra-particle medium. Computationally, the method consists of emitting $N_{r,i}$ rays from the i^{th} particle and finding the intersection of these rays with the nearest j^{th} particle that the ray intersects to compute an interaction (absorption or reflection) and continuing until all rays have exited the domain or the domain reaches thermal equilibrium. The parallel ray tracing is done by spatial decomposition. Each processor looks for intersections between a given ray and particles in the portion of the domain it is working on, with the ray handed off to neighboring particle if it exits the domain local to the processor without intersecting a particle. As an optimization the particles are stored in a kD-tree where the top level of the tree is built from equal sized spatial bins, allowing testing ray/bounding-box intersection to reduce the number of particles to check as shown in Figure 1.

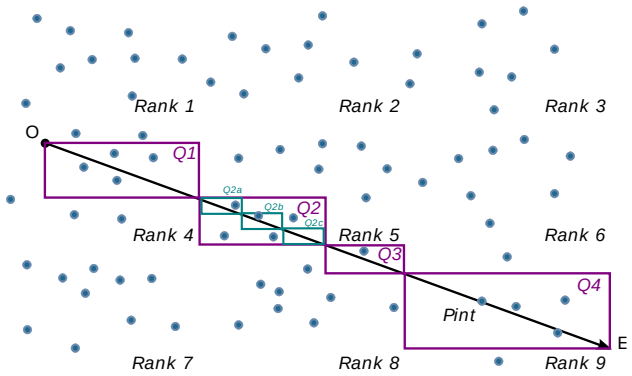

Figure 1: Spatial decomposition and particle grouping for ray/particle intersection test

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Validation and performance profiling was conducted on a benchmark problem provided by modest where the seen by a detector placed off-center relative to a radiation source with a participating medium is to be computed. The formulation used here should converge to the PMC method described by Modest when the medium is populated with particles; Figure 2 depicts the scenario and Figure 3, computed by the S3D code with zero velocity in the domain, shows the solution matching the solution given by Modest.

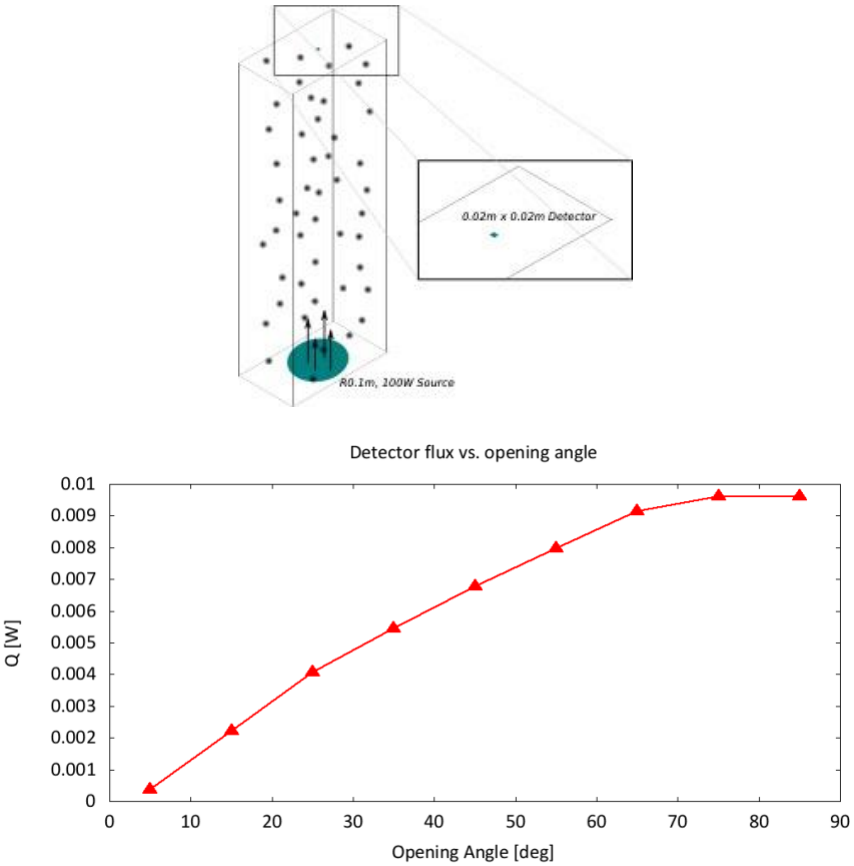

Figure 2:Validation case and simulation results

Performance profiling of the code for this problem for two scenarios that bookend performance: first, where the number of incident rays is orders of magnitude larger than the number of particles, and second, where the number of incident rays is small relative to the particle count and all particles emit irrespective of temperature. The relative effort of the various aspects of the problem are given in Table 2.

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Table 1: Division of computational time for scattering test case

Task	Execution time for case with large number of incident rays relative to particle count	Execution time fraction for large particle count
Emit incident rays	1%	0%
Relocating incident rays	3%	29%
Construct particle kD tree	1%	19%
Emit rays from particles	1%	16%
Traverse kD tree	5%	4%
Process tree leaves	50%	5%
Absorb rays	0%	0%
Balance of intersection detection	39%	40%
Maximum imbalance	89%	20%

Task 2: The software developed in the first portion of the project will be used to create datasets by UNSW. NREL will contribute computing time on *Peregrine* up to 3M conventional CPU hours and technical support to UNSW with respect to compilation, job submission. NREL will also provide storage for the datasets over the lifetime of this project.

The software developed in Task 1, known as "S3D-multiphase", was used to conduct simulations that demonstrated a robust two-way coupling between compressible DNS and point particles at a variety of Stokes numbers. The simulation environment is shown in Figure 3, below, and consists of a particle laden round jet issuing into a rectangular domain. This resulted in the first direct simulations of the interactions of turbulence, solar radiation, and chemistry in particulate flows. The simulations were performed in the US on DOE supercomputers and in Australia using national supercomputing resources.

These simulations established cutting-edge DNS databases for investigation of particle-laden flows with significant radiation effects: The DNS tool was applied using supercomputing resources at NREL and in Australia to establish a series of globally unique databases. These included a series of DNS of the experimental two-phase jets at Adelaide, achieving a world-first level of agreement between the model and experiment, enabled by combining accurate experimental boundary conditions and measurements with the highly accurate DNS code [12]. It also included the first DNS study of radiation interacting with soot particles with detailed soot and radiation models, corresponding to the interest in this system in the Adelaide team's hybrid solar-combustion receiver [13].

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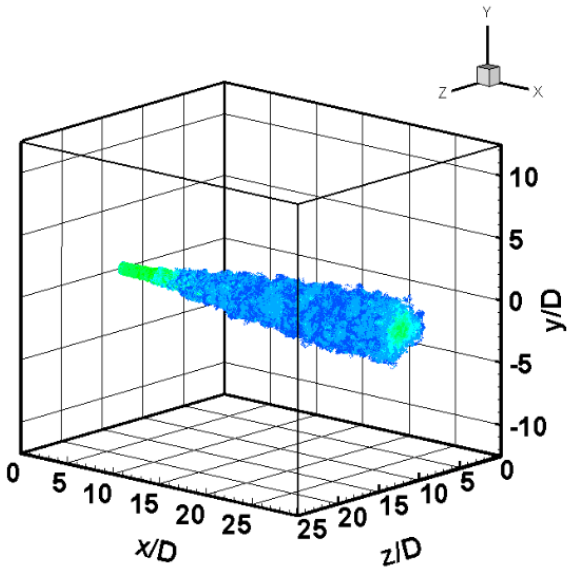

Figure 3: Schematics of the flow configuration

Using the first simulation conducted by UNSW with NREL support, the influence of Stokes number on the velocity and particle concentration distributions has been investigated. Three different Stokes numbers were simulated (0.3, 1.4 and 11.2). In the past, several efforts have been made to model the particle-laden flows in jet configuration. However, in all the studies, two basic assumptions have been utilized. Firstly, that the particles exit the nozzle with a uniform distribution, irrespective of the Stokes number. Secondly, almost all studies consider the initial velocities of the particles to be the same as local instantaneous fluid velocities. In these simulations, efforts were made to ensure that the initial conditions of carrier and the particle phase matched those of the recent experiments. Hence, to the best of our knowledge, this is the first attempt towards accurately modeling a particle-laden turbulent round jet using DNS with realistic initial conditions.

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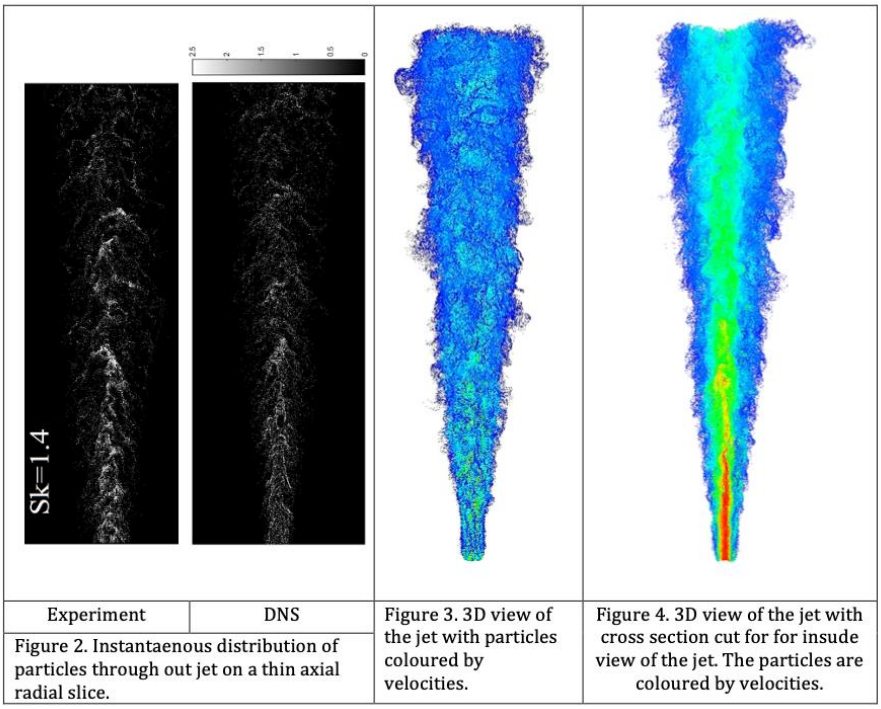

Figure 4: Comparison of observed vs. simulated jet particle structure

Figure 4 shows a qualitative comparison between the numerical results and experiment where the particle clusters have similar structure.

A key finding is that initial particle distribution at the nozzle exit plays important role in the jet development. Neglecting this effect may result in significant differences from real scenarios, particularly in the near to immediate field of the jet. This is of particular importance because of the models (for approximate, engineering design-cycle type calculations) that have been built on the previous high-fidelity simulations that have use simplistic initial particle distributions. These findings are discussed in a variety of conference papers [14-16].

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Overall, this project produced significant achievements enabled by the joint experimental and numerical investigations of underpinning phenomena relevant to solar thermochemical reactors with suspended particles. The CRADA work – specifically construction of very high fidelity simulation capability and datasets - supported development of modelling tools necessary to design new reactor concepts.

Subject Inventions Listing:

None

ROI #:

None

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