DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof. Reference herein to any social initiative (including but not limited to Diversity, Equity, and Inclusion (DEI); Community Benefits Plans (CBP); Justice 40; etc.) is made by the Author independent of any current requirement by the United States Government and does not constitute or imply endorsement, recommendation, or support by the United States Government or any agency thereof.

Cooperative Research and Development Agreement Final Report,

CRADA TC02358

February 3, 2023

Victor Castillo, Rapid CFD Using Machine Learning Algorithms

Innovations and Partnerships Office

Prepared by LLNL under Contract DE-AC52-07NA27344.

Lawrence Livermore National Laboratory

LLNL-TR-2012760

NNSA National Nuclear Security Administration

Rapid CFD Using Machine Learning Algorithms

Cooperative Research and Development Agreement Final Report
CRADA No. TC02358
Date Technical Work Ended: November 10, 2022

February 3, 2023

A. Parties

This project was a relationship between Lawrence Livermore National Security, LLC and Guardian Glass, LLC.

Lawrence Livermore National Security, LLC
Lawrence Livermore National Laboratory
7000 East Avenue
Livermore, CA 94550
Victor Castillo
Tel: (925) 424-5049
Email: castillo3@llnl.gov

Guardian Glass, LLC
14511 Romine Road
Carleton, MI 48117
Yousef Mohassab
Tel: (801) 386-0358
Email: ymohassab@guardian.com

This CRADA project was sponsored under the High-Performance Computing for Manufacturing (HPC4Mfg) Program of the Department of Energy's Advanced Manufacturing Office (AMO) within the Energy Efficiency and Renewable Energy (EERE) Office.

	Year 1		
Funding Type	Funds-in	*In-kind	Totals
Cleveland-Cliffs	$0	$75,000	$75,000
Dept. of Energy [EERE/AMO]	$300,000		$300,000
Totals			$375,000

B. Project Scope

This is a collaborative effort between Lawrence Livermore National Security, LLC as manager and operator of Lawrence Livermore National Laboratory ("LLNL") and Guardian Glass, LLC ("Guardian Glass") to develop a fast-running emulator of the reactive Computational Fluid Dynamics ("CFD") simulations needed to understand the complex reactions and flows in the glass melting, fining, and forming subprocesses. This CRADA project is sponsored under the High-Performance Computing for Manufacturing ("HPC4Mfg") Program of the Department of Energy's Advanced Manufacturing Office ("AMO") within the Energy Efficiency and Renewable Energy ("EERE") Office.

The project was originally designated as a twelve (12) month project. A No-cost Time Extension for this project extended the CRADA for five (5) months due to change in project focus by Guardian Glass management. It was later extended by two (2) months due to a family medical emergency of the LLNL PI. The project activities were concluded on November 10, 2022.

The CRADA consisted of six (6) major tasks and the following six (6) major deliverables:

Deliverable 1: Guardian Glass will provide initial CFD simulation results which will be used as a template to support workflow development. These will be in a common format such as HDF5, VTK, CSV, etc. (Project Month 2)

Deliverable 2: LLNL will provide the Experimental Design for simulation study. (Project Month 3)

Deliverable 3: Guardian Glass will provide CFD result files (HDF5 or VTK) and post-processed quantities to LLNL. (Project Month 6)

Deliverable 4: LLNL will provide an initial reduced-order model that can be compared to simulation results. The best machine learning based algorithm is also provided. This will be as a computer routine that will execute on a game-class workstation or laptop. (Project Month 9)

Deliverable 5: Guardian Glass will provide results of additional simulations and comparisons to the initial reduced-order model. Guardian Glass will also access the accuracy of the reduced-order model and provide information regarding the usability in a production setting. (Project Month 11)

Deliverable 6: The Final Report as required under Article X of the CRADA. (End of Project)

All project elements were successfully completed. The result was a fast-running surrogate model that was trained on simulations of a production glass furnace under a variety of conditions. This included the heat distribution of several gas burners and five other control variables. The

surrogate model was produced with a python-based graphical user interface (GUI) and delivered. (Software release: Guardian Glass ROM; CP Number CP02649). This surrogate model was validated by comparison with simulations conducted by Guardian Glass and demonstrated excellent performance.

We have provided three technical reports to Guardian Glass:

- Guardian Glass Project Mid-term Update 1 (LLNL-TR-833087); Vic Castillo, Yeping Hu; 3/25/2022: V3 and V4 sampling strategies
- Guardian Glass Project Mid-term Update 2 (LLNL-TR-836879); Yeping Hu, Vic Castillo; 5/17/2022: Data preprocessing and feature detection
- Guardian Glass Project Mid-term Update 3 (LLNL-TR-836880); Yeping Hu, Vic Castillo; 6/9/2022: ML methods
- Rapid CFD Project; Guardian Glass: Project Summary (LLNL-TR-836880); Vic Castillo, Yeping Hu; 11/17/2022: Updated with validation results

Property: No property was exchanged during the project.

Liens: There are no outstanding liens.

C. Technical Accomplishments

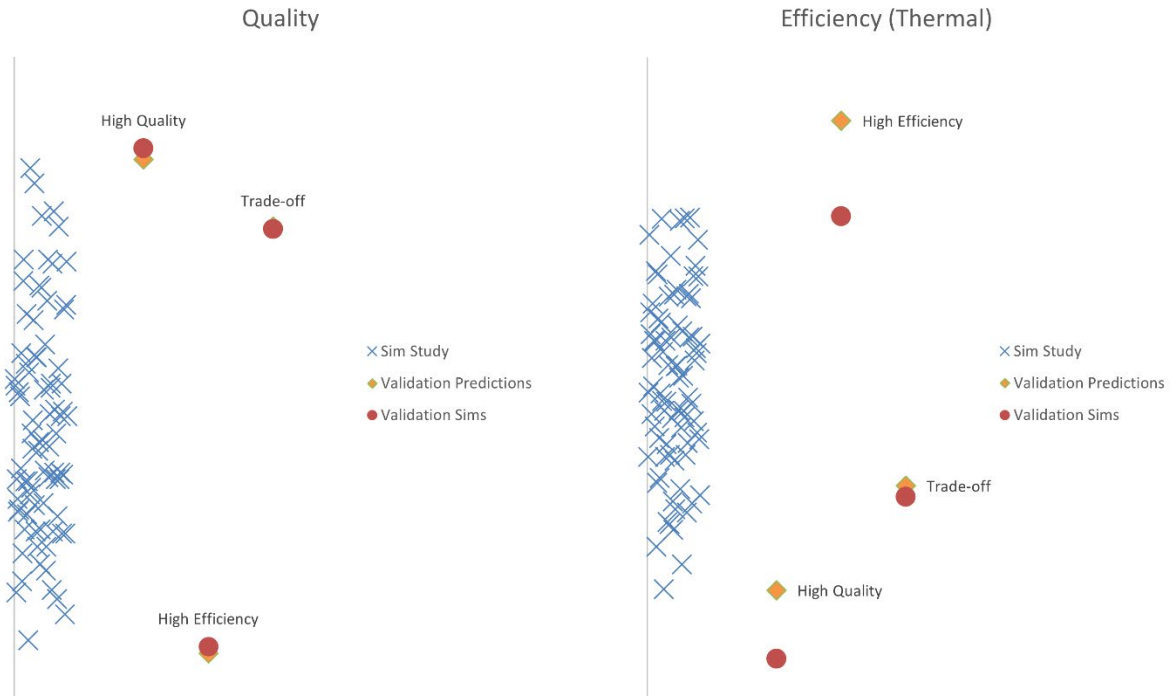
This project had six key tasks including Task 6 ... the final reports. Task 1 was a deep dive into the production system pain points and key variables. This led to an eleven-dimensional design (Task 2) with 116 simulations that were completed in December 2021 (Task 3). Note that each run took about 72 hours on the Guardian cluster. Unfortunately, priorities and Guardian Glass changed at this point and the key variables and ranges needed to be changed. To address this, all parties agreed to a 5-month No Cost Term Extension and Tasks 2 and 3 were repeated (Tasks 2′ and 3′). The following design, referred to as V4, leveraged several of the original set and added 75 simulations to sample a 9-dimensional design space. The V4 simulations were completed by April 2022.

Analysis of the V4 simulations revealed an anomalous region that had many failed simulations. Further analysis could not isolate the good from the bad part of this region which appeared like a mine field. There were a few ideas why this region was somewhat chaotic but eventually engaged with the simulation tool provider who found and error in the software. This was quickly fixed by the simulation software vendor. Afterwards, simulations in that region not only had good performance, but they also had the best. These involved atypical port configurations and may influence future production conditions.

The reduced-order model was developed (Task 4) from a 2D slices of the temperature and velocity fields along the side-to-side center plane (xz) and parallel to the surface plane (xy) near

the top and bottom of the tank. We used a combination of GNNs and non-linear regression methods and were able to achieve models with very low loss.

We used the models to make predictions of run conditions that would produce 1) high product quality, 2) high thermal efficiency, and 3) a trade-off that sacrificed some quality for increased thermal efficiency (multi-attribute optimization). The first two were actually extrapolations of conditions outside of the V4 study. The Guardian team ran simulation of these cases to validate the results (Task 5) and confirmed the predictions.



D. Expected Economic Impact

D.1 Specific Benefits

Benefits to DOE: This benefits the DOE by directly supporting the mission of the EERE Advanced Manufacturing Office (AMO) through its High-Performance Computing for Manufacturing program.

This project advances the goals of the HPC4Mfg program in three ways: 1) a reduced order glass furnace prediction model implemented into manufacturing for use by plant personnel and as the basis for an improved control scheme will lead to higher energy productivity and reduced emissions in the energy-intensive flat glass industry, 2) it opens up a collaboration between Guardian Glass and LLNL to leverage respective areas of expertise in achieving the goal of energy reduction, and 3) it will improve the manufacturing efficiency of a variety of glass formulations and glass furnace designs in the US. The knowledge transferred from LLNL

model reduction experts to Guardian Glass also supports HPC4Mfg goals. The knowledge transfer will ensure the results of the program will be more broadly implemented throughout the company, and that HPC techniques to improve manufacturing will become ingrained in the manufacturing culture of this industry and support the long-term competitive position of the US in this area.

Benefits to Industry: Through this CRADA project, HPC techniques to improve manufacturing will become ingrained in the manufacturing culture of this industry and support the long-term competitive position of the US in this area.
Once accredited, the reduced-order model can be used to directly inform operators or process control systems in real-time, thus allowing for early process intervention that can minimize the risk of process upsets during typical furnace operation. Additionally, the speed of computation for the machine learning model will enable energy minimization studies given logical constraints, i.e., preserved glass quality and throughput. Put another way, this work will make it possible to identify ideal process input targets. A modest estimate on the potential impact would be a 5% reduction in natural gas consumption, which, if applied across all U.S. float production lines, would save roughly 2.5 million GJ per year while reducing CO_2 emissions by roughly 130,000 metric tons

E. Participant Contribution

The Participant provided subject matter expertise throughout CRADA execution with weekly or biweekly meetings. Additionally, the Participant run simulations using the GTM-X solver, a commercial CFD code developed by CelSian Glass & Solar BV. These simulations couple the combustion gas space and glass melt and can take in excess of two weeks to complete running on 24 cores.

F. Documents/Reference List

Reports: Progress presentations were given quarterly to the Participant's management. Additionally, technical reports were provided regarding the flow feature analysis and model development:

- Guardian Glass Project Mid-term Update 1 (LLNL-TR-833087); Vic Castillo, Yeping Hu; 3/25/2022: V3 and V4 sampling strategies
- Guardian Glass Project Mid-term Update 2 (LLNL-TR-836879); Yeping Hu, Vic Castillo; 5/17/2022: Data preprocessing and feature detection
- Guardian Glass Project Mid-term Update 3 (LLNL-TR-836880); Yeping Hu, Vic Castillo; 6/9/2022: ML methods
- Rapid CFD Project; Guardian Glass: Project Summary (LLNL-TR-836880); Vic Castillo, Yeping Hu; 11/17/2022: Updated with validation results

Copyright Activity
We developed a custom reduced-order model (ROM) with a Graphical User Interface (GUI) based on methods developed from the FY21 AMO ML Capability Project (Title: "Generalizable

Scientific Machine Learning Tool Suite for Manufacturing"; Tracking ID: CAP-1-21-26488). The software was developed in python and leveraged open-source tools such as PyTorch and pyvista. We released an "inference version" of the code to Guardian Glass in December 2022 (Software release title: Guardian Glass ROM; CP Number CP02649).

Subject Inventions

No inventions were created.

Background Intellectual Property

LLNL disclosed the following Background Intellectual Property for this project: See Copyright Activity

Participant disclosed the following Background Intellectual Property for this project: None.