Electronic Supplementary Material (ESI) for Energy & Environmental Science

Supplementary Information

Aerosol Generation by Reactive Boiling Ejection of Molten Cellulose

Andrew R.Teixeira, Kyle G. Mooney, Jacob S. Kruger, C. Luke Williams, Wieslaw J.Suszynski, Lanny D. Schmidt, David P. Schmidt, Paul J. Dauenhauer

Overview of Supplementary Information

The supplementary information consists of the following files.

- Supplementary Information and Figures (this document)
- Supplementary Video 1 – Cellulose Ejection
- Supplementary Video 2 – Multiple Cellulose Ejection
- Supplementary Video 3 – Sucrose Ejection and Mechanism
- Supplementary Video 4 – CFD Ejection Simulation 1
- Supplementary Video 5 – CFD Ejection Simulation 2
- Supplementary Video 6 – CFD Ejection Simulation 3
- Supplementary Video 7 – Molten, Bubbling Lignin

Supplementary Videos

The following is a brief description of each Video file.

Video S1 – Cellulose Ejection

Video S1 depicts a droplet of intermediate cellulose liquid on a 700 °C surface ejecting a liquid droplet. The ejected droplet is visible in multiple frames as it slows down while passing through the surrounding nitrogen gas. Frames from this video were used to produce Figure 3A. A brightness and contrast adjustment has been applied to all of the frames of the video uniformly using video software Virtualdub 1.9.9.

Video S2 – Multiple Cellulose Ejections

Video S2 depicts a droplet of intermediate cellulose liquid on a 700 °C surface near the end of its lifetime. Multiple ejections are visible within the focused region between the front and back of the particle. Ejections are visible as white streaks for 1-3 frames. Frames from this Video were used to produce Figure 1B. A brightness and contrast adjustment has been applied to all of the frames of the video equally using software Virtualdub 1.9.9. Frames were then differenced using the image subtraction technique in ImageJ as described earlier. The two sequences are displayed side by side. The original video frames are visible in Figure S5.

Video S3 – Sucrose Ejection and Mechanism

Video S3 depicts a droplet of molten sucrose liquid on 650 °C Fecralloy after it has melted to a liquid. A vapor bubble grows in size and rises to the upper right of the liquid droplet. Subsequent rupture of the liquid layer between the vapor bubble and the external gas results in the formation of a jet followed by fragmentation to an ejected droplet. A brightness and contrast adjustment has been applied to all of the frames of the video equally using software Virtualdub 1.9.9.

Video S4 – CFD Ejection Simulation Case 1

Animation of the simulation shown in Figure S13. (R_B=15 µm, R_{drop}=113 µm, γ=10^{-5} N/m, µ=10^{-5} kg/m·s)

Video S5 – CFD Ejection Simulation Case 2

Animation of the simulation shown in Figure 8. (R_B=15 µm, R_{drop}=113 µm, γ=$5\cdot10^{-6}$ N/m, µ=10^{-6} kg/m·s)

Video S6 – CFD Ejection Simulation Case 3

Animation of the simulation shown in Figure S12. (R_B=15 µm, R_{drop}=113 µm, γ=$5\cdot10^{-6}$ N/m, µ=10^{-5} kg/m·s)

Video S7 – Molten, Bubbling Lignin

Particles of lignin were pressed and sieved to 300 µm in diameter then pyrolyzing on a 700°C flat α-alumina surface via a liquid intermediate. An evolving liquid is observed rising from the bottom of the particle to the top as time progresses.

Supplementary Figures

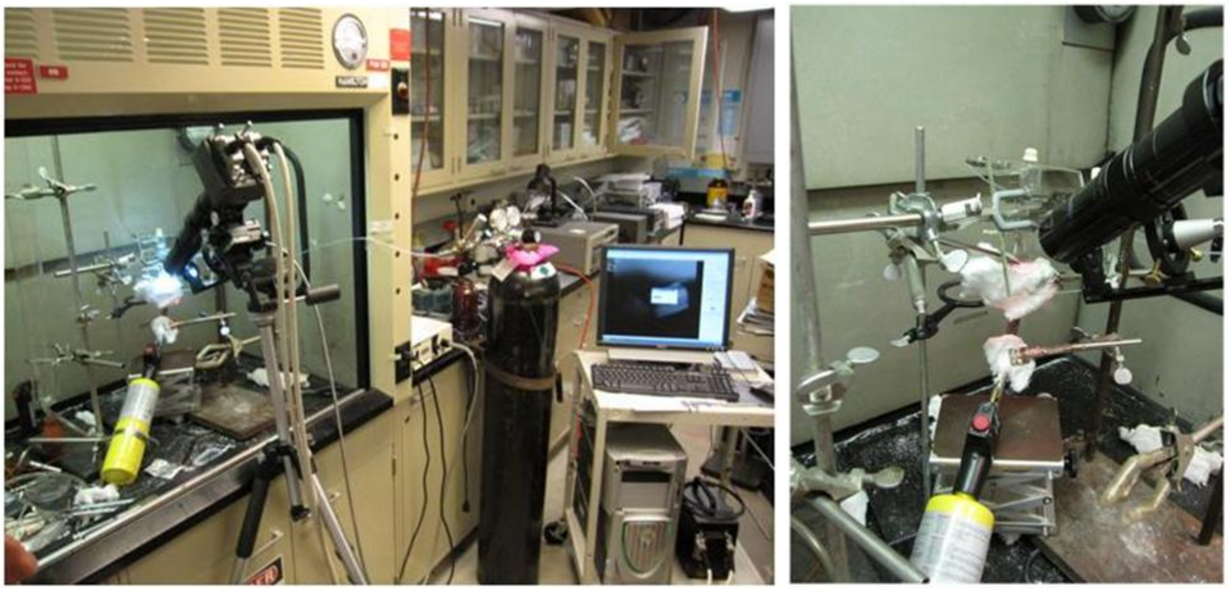

Figure S1. Experimental Setup for High Temperature Particle Visualization. Left. The high speed photography camera directly connects to a personal computer. Nitrogen gas is supplied to the pyrolysis experiment by a high pressure gas cylinder and controlled with a gas metering valve. Right: The high temperature surface is held in place by a metal cylinder supported with clamps and wrapped in white ceramic insulation. The assembly is heated from below by a MAPP torch capable of moving up and down to control the ceramic surface temperature. A quartz tube is held in place above the ceramic surface to provide nitrogen gas and particles to the surface in an inert environment. Lighting is provided from the right of the camera. A panel of glass is held in place between the camera lens and the surface.

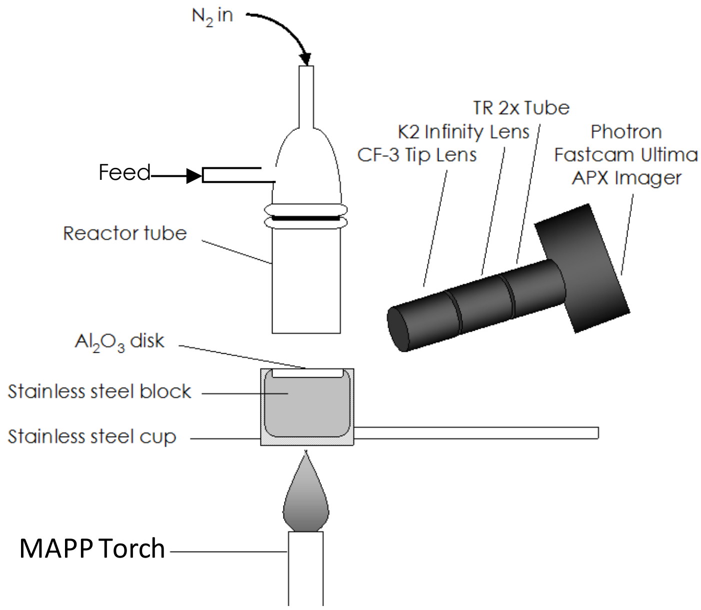

Figure S2. Schematic of the aerosol apparatus and system using an Al_2O_3 disk.

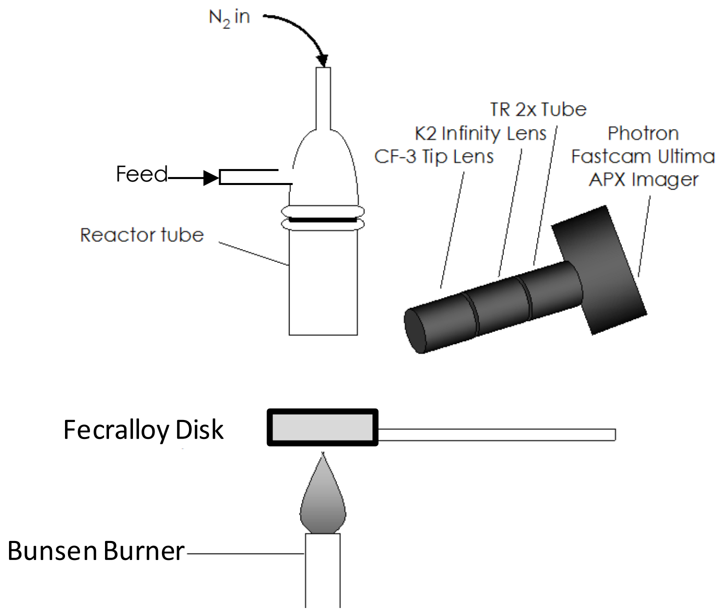

Figure S3. Schematic of the aerosol apparatus and system using a Fecralloy disk.

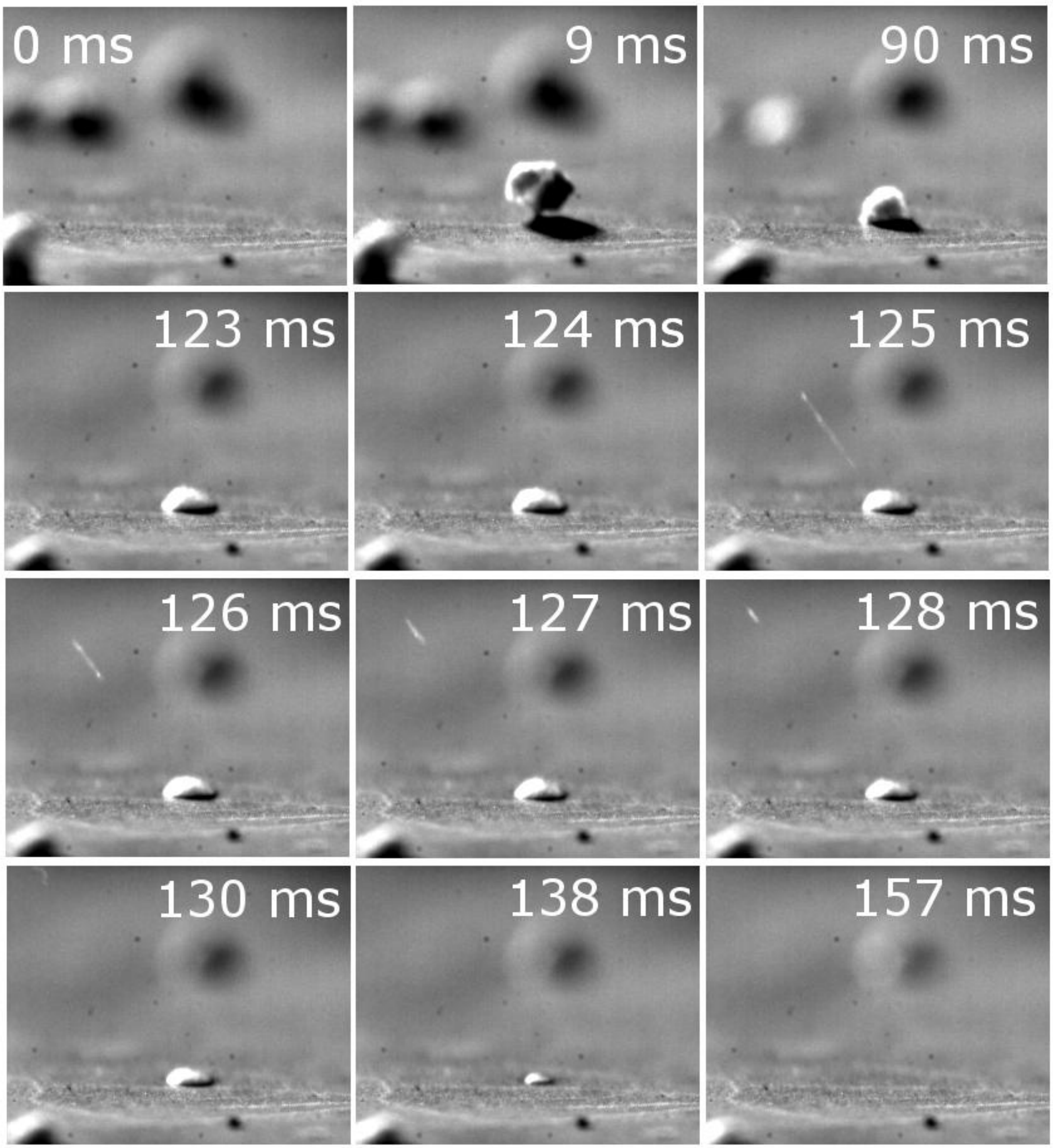

Figure S4. Droplet ejection from Intermediate Liquid Cellulose. A particle of cellulose (300 micron diameter) drops on a 700°C α-alumina surface (9 ms) and decomposes to a liquid intermediate. Droplet ejection is initiated (124 ms), and the ejected droplet is observed as a streak (125 ms). Frames 123-127 comprise Figure 3A of the manuscript.

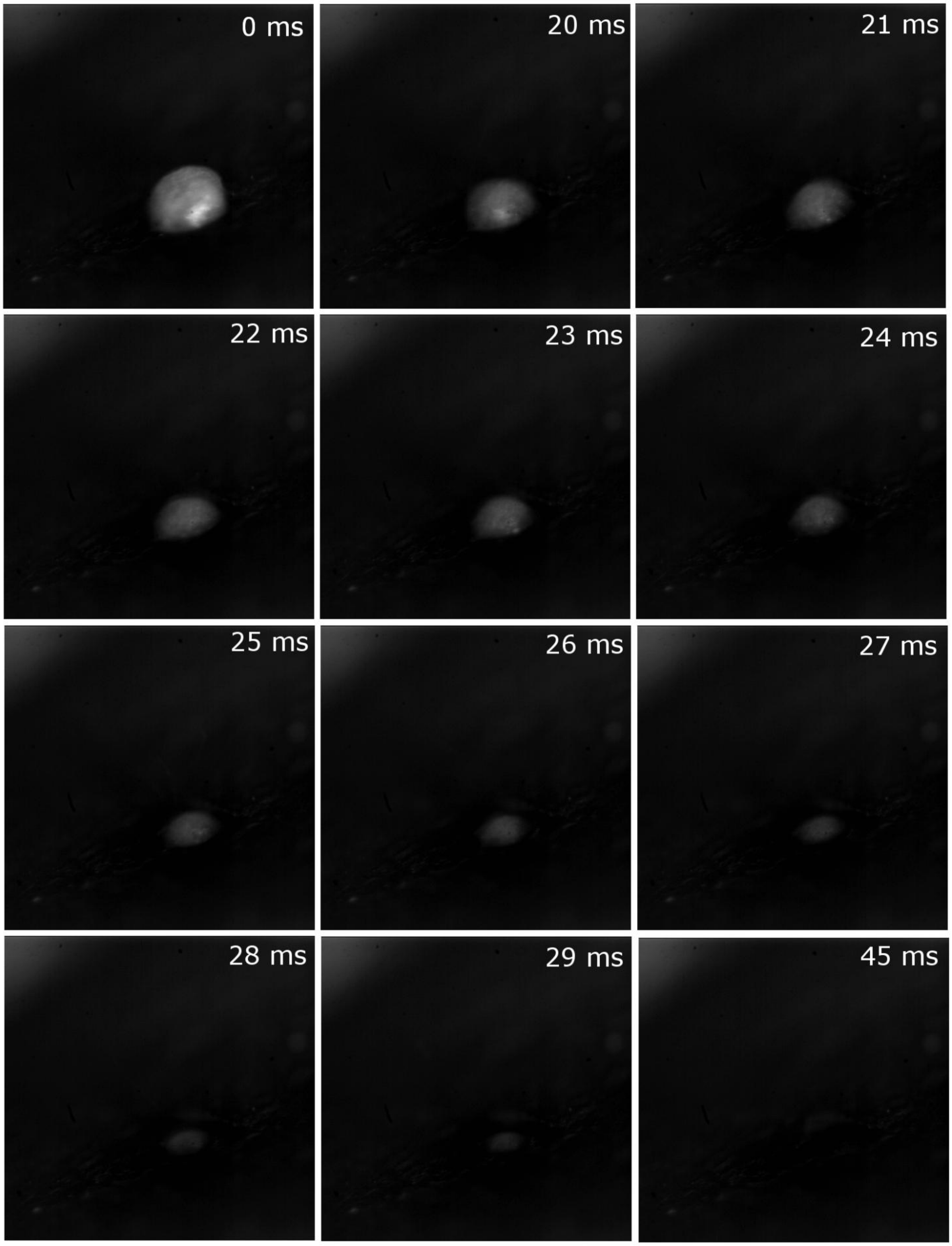

Figure S5. Multiple Drop Ejection from Liquid Intermediate Cellulose, Original Photography. A particle of liquid intermediate cellulose (250 micron diameter) on a 700°C α-alumina surface exhibits multiple ejections. All frames are derived from the original photography.

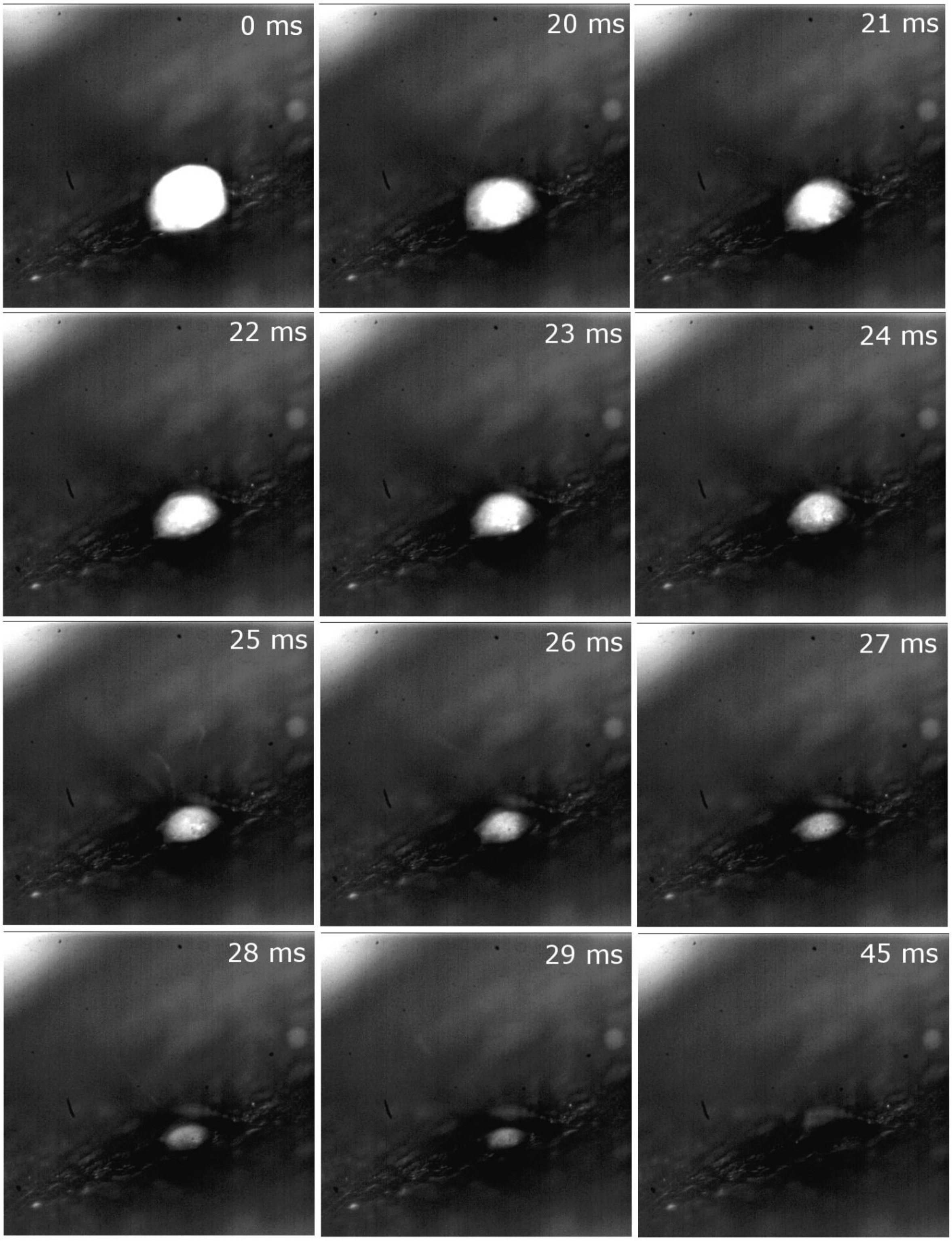

Figure S6. Multiple Drop Ejection from Liquid Intermediate Cellulose. A particle of liquid intermediate cellulose (250 micron diameter) on a 700°C α-alumina surface exhibits multiple ejections. The image has been contrast and brightness adjusted equally over the entire set; the original frames are visible in Figure S5.

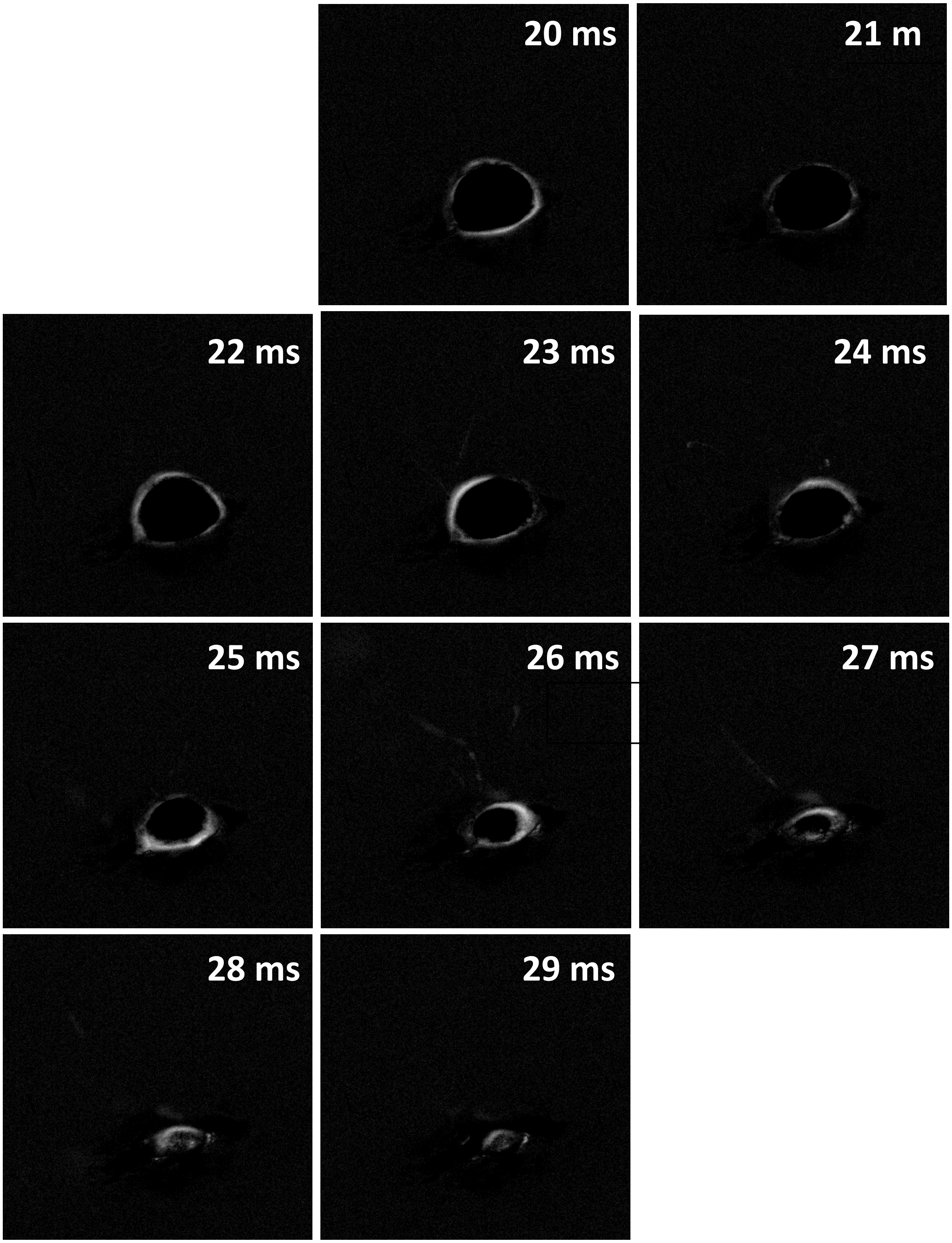

Figure S7. Multiple Drop Ejection from Liquid Intermediate Cellulose, Differenced. A particle of liquid intermediate cellulose (250 micron diameter) on a 700°C α-alumina surface exhibits multiple ejections. The image has been contrast and brightness adjusted equally over the entire set as observed in Figure S5.

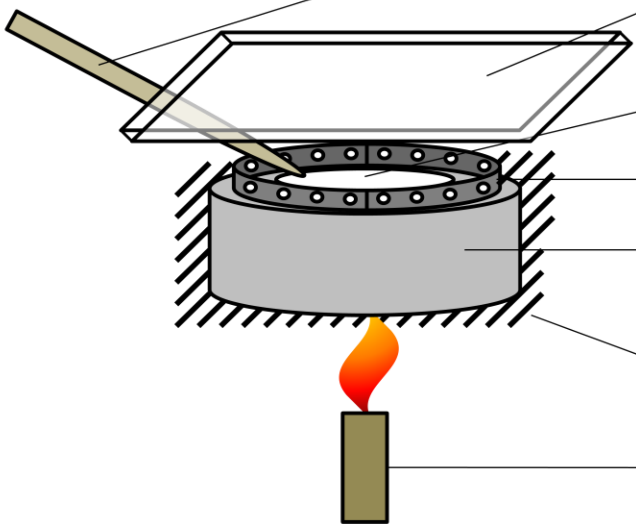

Figure S8. Aerosol Collection Apparatus. An α-alumina disk rests within a stainless steel cup encased in a ceramic insulation. Reaction surface temperatures are maintained at 700°C by use of a MAPP torch from below. As aerosols form, they adhere to the inclined glass slide.

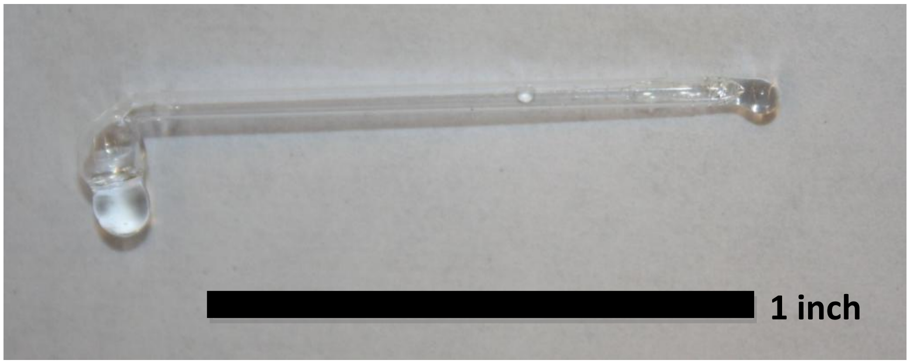

Figure S9. Custom-made Pyrolysis Tube. A custom-built pyrolysis tube used to generate the data in Figure 5B was made using a 9” Pasteur pipet, torch, and a tank of nitrogen. Particles of solid levoglucosan were placed within the pipet within an inert atmosphere, and the ends of the glass tube were sealed. The clear colorless liquid visible within the glass tube is pyrolyzed and reacted levoglucosan.

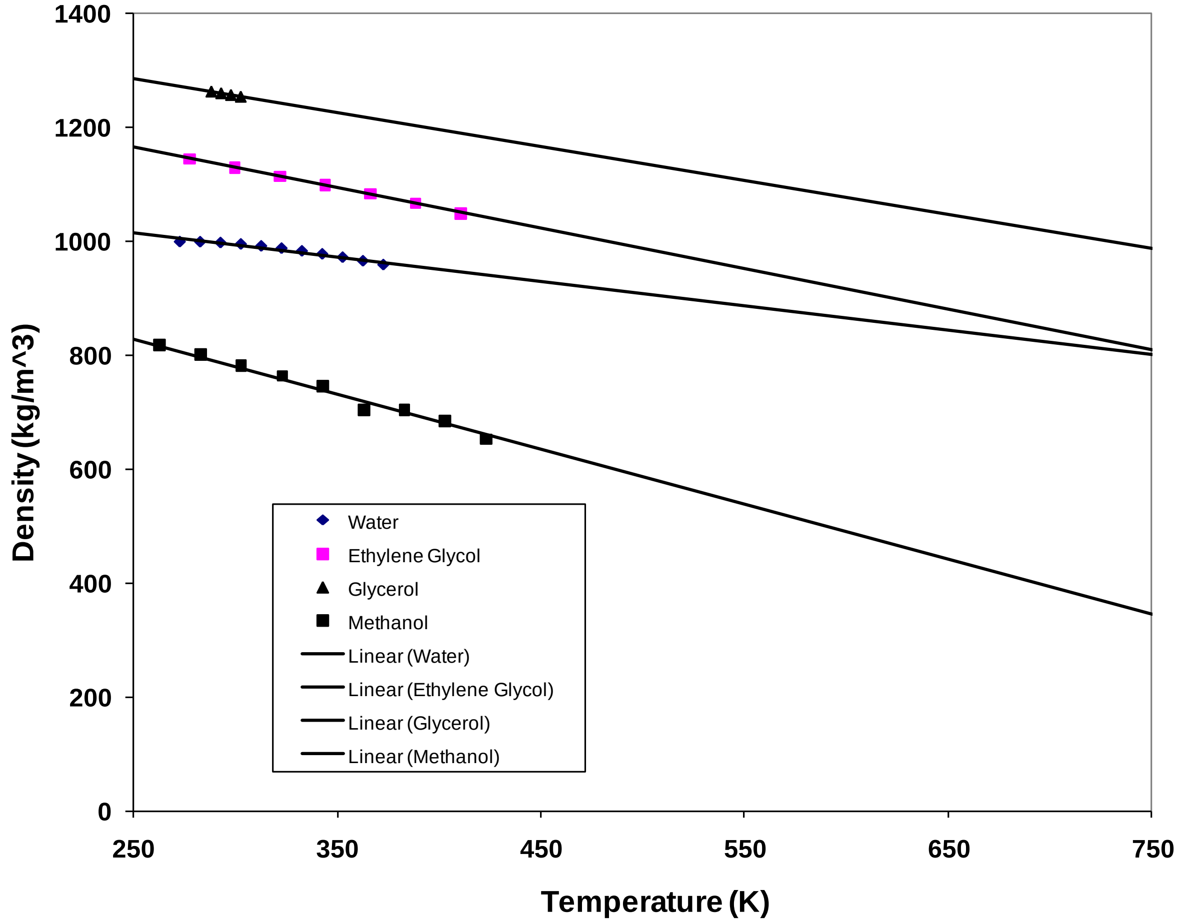

Figure S10. Prediction of Intermediate Liquid Cellulose Density. The density of the intermediate liquid cellulose has been predicted by extrapolation of oxygenated hydrocarbons and water below their boiling point to 750 K.

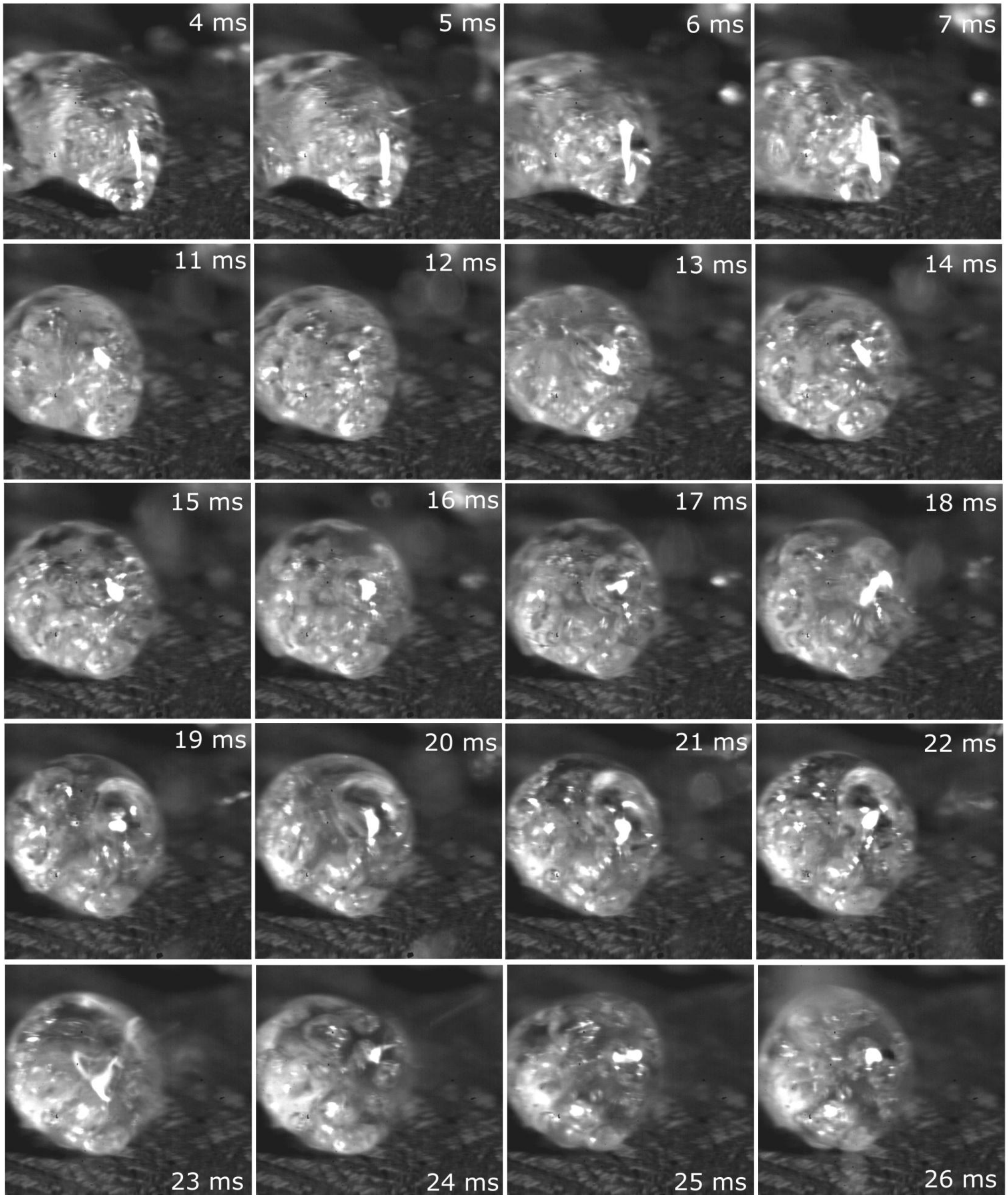

Figure S11. Sucrose Ejection on 650°C Fecralloy. Solid carbohydrate (β-D-fructofuranosyl-α-D-glucopyranoside) of 800 micron diameter on a 650°C Fecralloy surface (0 ms – not shown) melts and decomposes through a liquid intermediate. Bubble formation (19-22 ms) is followed by jet formation (23 ms) and subsequent particle ejection observed as a streak (24 ms). The jet observed at Frame 5 ms comprises Figure 6A. Frames are extracted from Supplementary Video S3.

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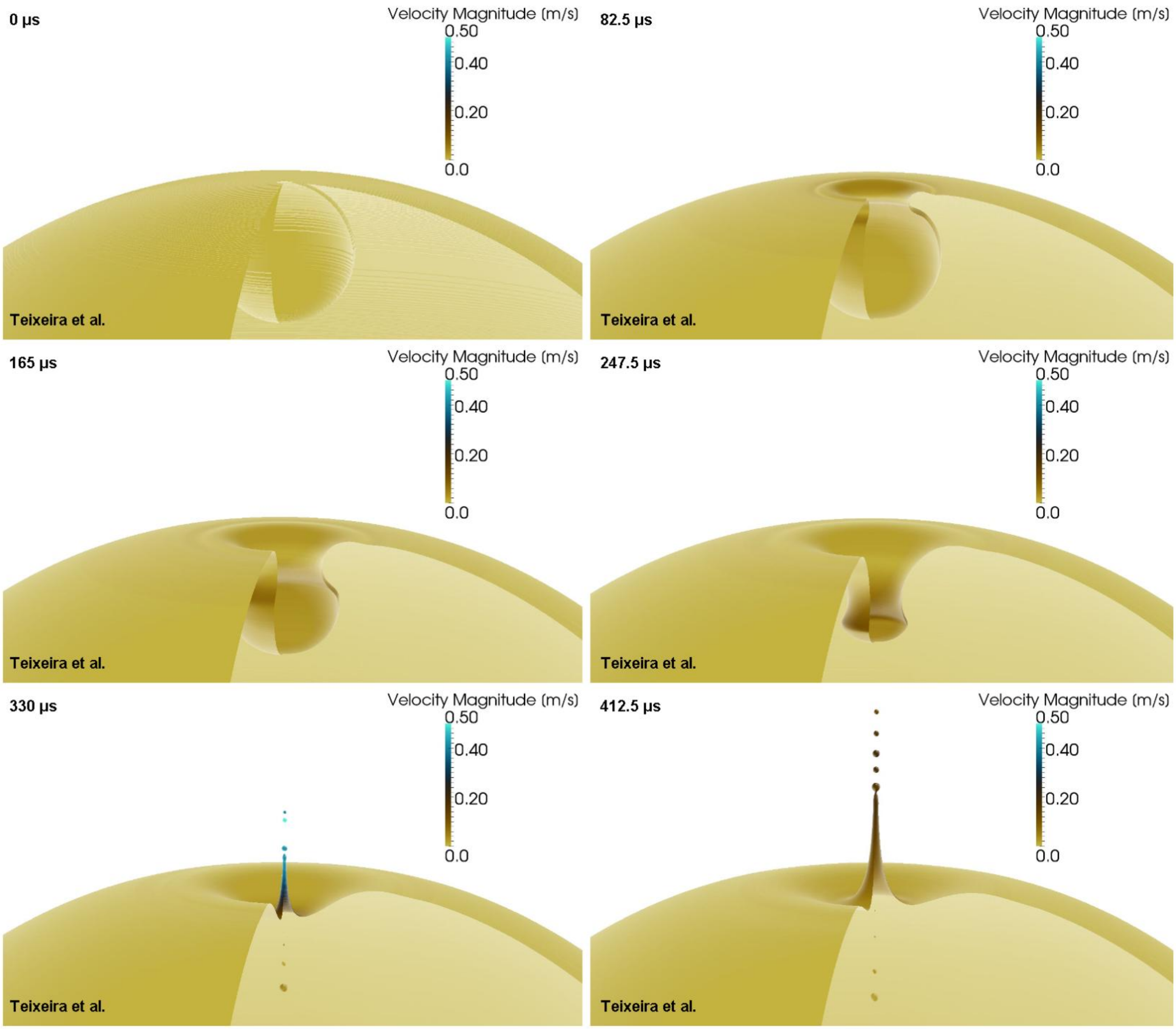

Figure S12. Supporting Simulation 3. Simulated bubble collapse and liquid jet formation depicting a 270° revolved α=0.5 iso-surface colored by velocity magnitude (R_B=15 µm, R_{drop}=113 µm, γ=5·10^{-6} N/m, µ=10^{-5} kg/m·s).

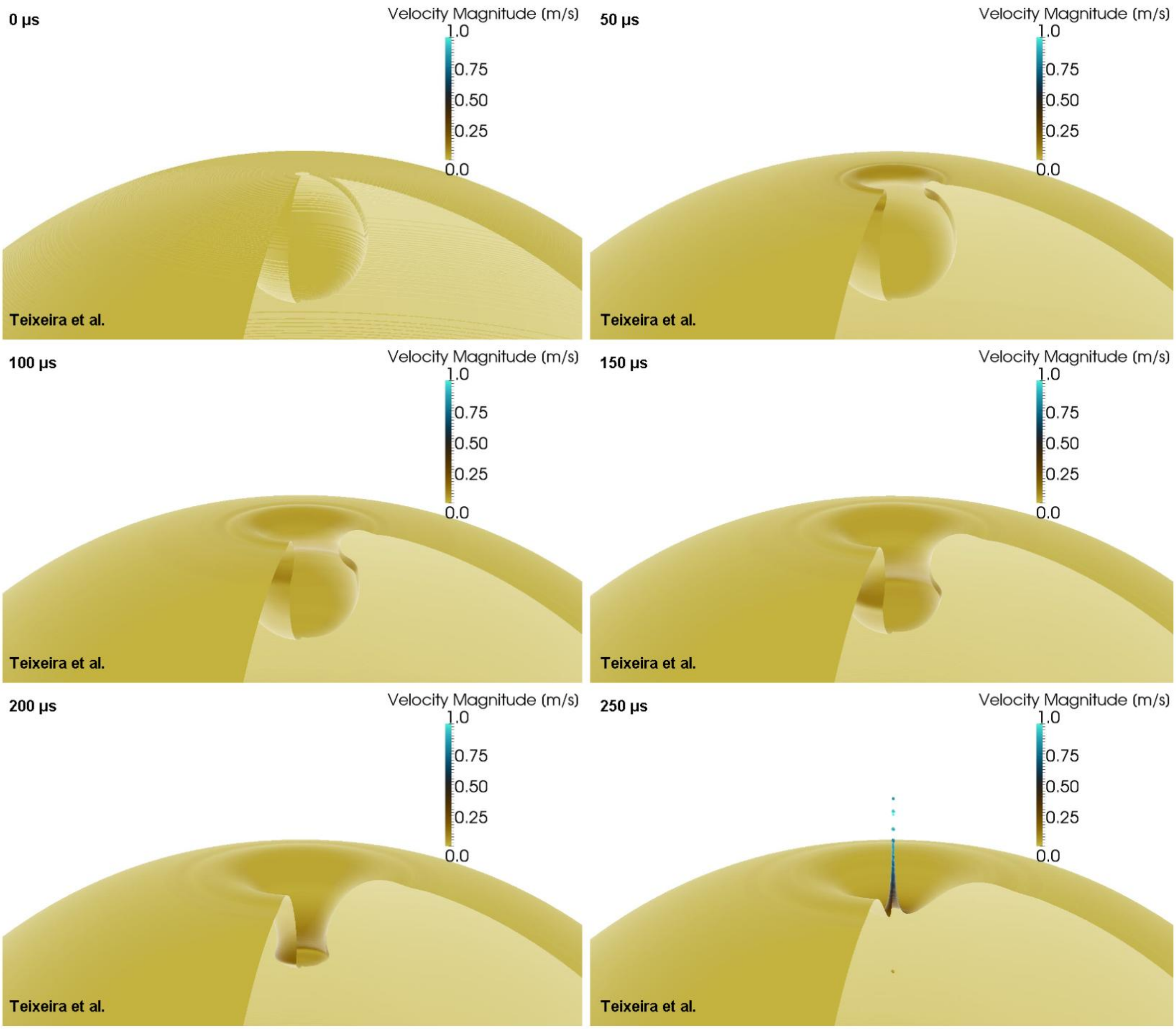

Figure S13. Supporting Simulation 1. Simulated bubble collapse and liquid jet formation depicting a 270° revolved α=0.5 iso-surface colored by velocity magnitude (R_B=15 µm, R_{drop}=113 µm, γ=10^{-5} N/m, µ=10^{-5} kg/m·s).

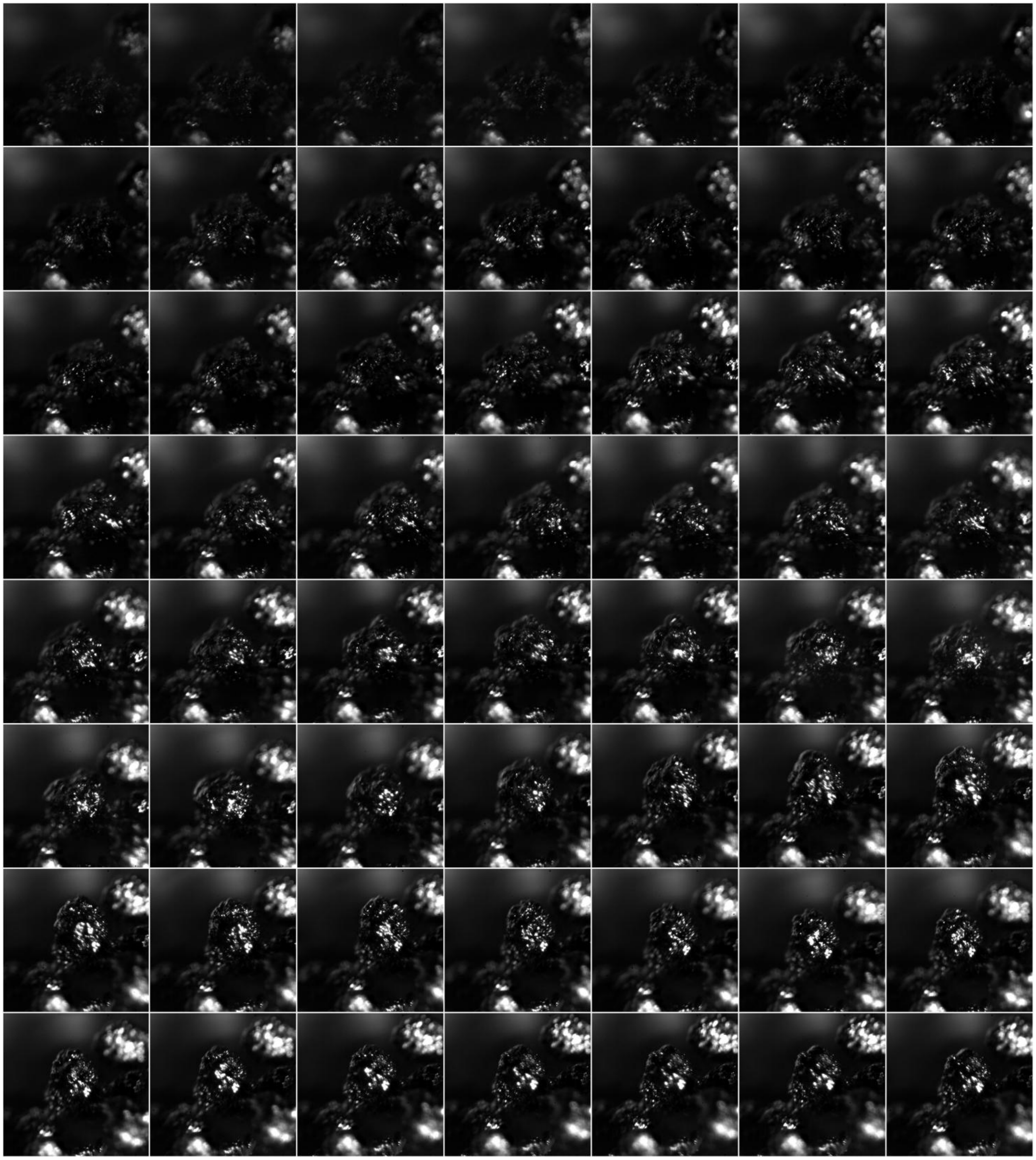

Figure S14. Molten Lignin Intermediate. Particles of lignin were pressed and sieved to 300 μm in diameter then pyrolyzed on a 700°C flat α-alumina surface via a liquid intermediate. The full video can be observed in Video S7†. An evolving liquid interface is observed rising from the bottom of the particle to the top as time progresses. Time between frames = 4 ms.