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Droplet-Size Distribution Effects on Urea–Water Spray Evaporation and Decomposition: Knowledge of Sauter Mean Diameter (SMD) is not Sufficient

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Abstract

Urea water solution is widely used in selective catalytic reduction systems to reduce nitrogen oxide emissions. Urea decomposes via thermolysis and hydrolysis to produce ammonia, which reacts on the catalyst to form non-toxic gases, while solid residues formed during decomposition may affect system performance. A stand-alone reduced model is used to investigate spray decomposition, enabling systematic analysis of droplet size distribution effects independent of full flow-field complexity. The model is based on a progress-variable formulation derived from detailed one-dimensional droplet simulations with comprehensive chemistry over a wide range of temperatures. A parcel-based approach represents arbitrary droplet size distributions. The influence of droplet size, temperature, and distribution shape on ammonia formation and residue production is quantified. Distributions with identical Sauter mean diameter are compared to assess its validity. The results show significant differences in ammonia release and residue formation. These differences are strongly temperature dependent and demonstrate that the Sauter mean diameter alone is insufficient to characterize sprays for accurate decomposition modeling. A strong positive correlation between ammonia production and residue formation is observed. The findings show that representing the full droplet size distribution is essential for accurate prediction of ammonia availability and deposit formation.

1. Introduction

Emissions of NO_x have a harmful impact on human health and an indirect effect on climate change, and contribute to the formation of acid rain [1, 2]. Consequently, increasingly stringent Euro emission standards have been introduced to limit NO_x emissions from combustion engines [3]. Among the available after treatment technologies, selective catalytic reduction (SCR) using ammonia has been shown to be highly effective [4]. In this process, ammonia reacts with NO_x to form non-toxic products [5].

Because ammonia is toxic and corrosive, it is generated on-board through the thermal decomposition of urea supplied as an aqueous urea-water solution (UWS) [6].

In industrial SCR applications, a standardized 32.5% urea-water solution is injected into the exhaust system [7]. Urea CO(NH₂)₂ serves as a source of NH₃, which reacts with NO_x in the SCR process. The UWS-SCR process can be divided into three successive stages: (i) spray injection and droplet evaporation, during which urea decomposition begins; (ii) wall impingement and liquid-film formation; and (iii) gas-phase transport carries decomposition products and solid residuals, with the latter in particles, to the catalyst monolith, as schematically illustrated in Fig. 1.

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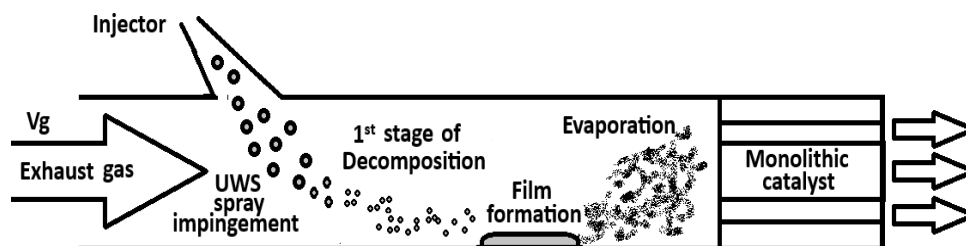


Fig. 1. Schematic representation of the urea decomposition process in an SCR system. The first stage corresponds to droplet evaporation and decomposition prior to wall impingement.

In recent decades, substantial progress has been made in understanding the chemical kinetics governing urea decomposition. Early studies focused on fundamental thermodynamic and kinetic descriptions of urea thermolysis and associated water evaporation mechanisms [8, 9, 10]. These works provided essential insights into reaction pathways, but offered limited accuracy in capturing multiphase interactions and the transient evolution of droplets under realistic exhaust conditions.

Subsequent modeling efforts extended these foundational descriptions by incorporating multiphase transport, spray dynamics, and droplet-scale heat and mass transfer. Detailed kinetic and CFD-based approaches were proposed to describe urea hydrolysis, decomposition reactions, and droplet evaporation in SCR systems [11, 12, 13]. To mitigate the high computational cost of such models, empirical and semi-empirical formulations were also developed, providing simplified correlations calibrated against experimental data [14].

More recent studies combine high-fidelity CFD with detailed chemical kinetics to accurately resolve droplet evaporation, urea melting, and multi-step reaction pathways under engine-relevant conditions [15, 16, 10]. In parallel, hybrid fluid–solid approaches have been introduced to capture wall-film formation and deposit growth by coupling spray dynamics, evaporation, and surface chemistry [17, 18]. Reduced-empirical models have also gained attention as computationally efficient alternatives, suitable for large-scale simulations, control strategies, and real-time applications [19]. Experimental–numerical studies further support these developments by validating decomposition mechanisms and deposit behavior under realistic SCR conditions [20, 21, 22].

Despite these advances, modeling UWS decomposition in SCR systems remains challenging due to the strongly coupled multi-phase and multi-physics nature of the process. The wide range of time scales-

from rapid droplet evaporation to slower film and deposit formation-renders fully resolved three-dimensional simulations computationally demanding [15, 16, 23]. In addition, deposits that form on mixers, pipes, and catalyst surfaces can significantly deteriorate the performance of SCR, yet these effects are often simplified or neglected in practical simulations [19]. The limited availability of detailed experimental data on the droplet and film-scale further complicates model validation and parameterization [24]. These limitations motivate the development of models that balance physical fidelity with computational efficiency.

To address these challenges, several reduced modeling approaches have been developed in our previous works. In [25], a multiphase one-dimensional symmetry framework was introduced for UWS droplets and films under SCR conditions, combining gas-phase chemistry with droplet evaporation and decomposition [26]. The gas-phase dynamics were reduced using the Reaction-Diffusion Manifold (REDIM) method, while the droplet and film evolution were described by a polynomial model. Building on this framework, [27] proposed an improved reduced model that captures the complete evaporation and decomposition process using only three parameters, enabling accurate predictions of droplet size evolution and species release at significantly reduced computational cost. To extend this formulation to a broader region of interest (ROI) and account for droplet-size and temperature-dependent decomposition behavior, a tabulation strategy was introduced in [28], in which detailed one-dimensional droplet solutions are precomputed as functions of initial droplet size, ambient temperature, and a progress variable describing the coupled evaporation and decomposition processes, while remaining compatible with Lagrangian parcel-based CFD spray simulations [29].

The present study focuses on the pre-impingement stage of UWS decomposition, in which the injected droplets evaporate and decompose before reaching the wall (see Fig. 1). In CFD simulations, droplet size distributions are commonly represented using a Rosin-Rammler function, whose parameters provide a simple and widely adopted description of atomizer-generated polydisperse sprays [30]. This approach is considered here using application-relevant parameters and is compared with the Sauter Mean Diameter (SMD) [31], which represents the diameter of a monodisperse droplet with the same volume-to-surface-area ratio as a polydisperse spray and is widely used to characterize processes dominated by evaporation [32, 33]. In addition, a bimodal distribution (double-hump) is examined to account for the presence of satellite droplets [34]. The influence of different droplet size distributions on the completeness of urea decomposition is assessed by analyzing ammonia release and solid residue formation under application-relevant conditions, and the validity of SMD-based and Rosin-Rammler-based representations is discussed.

By focusing specifically on the pre-impingement stage, this study highlights how even subtle variations in droplet-size distributions beyond what SMD captures directly influence ammonia availability and solid residual formation, providing new insight into the initial conditions that shape subsequent wall-film evolution and SCR reactions.

2. Modelling

2.1. Modeling assumptions and simplifications

The model considered for the decomposition of urea-water solutions relies on several key assumptions. First, the spray is considered to consist of sparsely and homogeneously distributed spherical droplets with stagnant surrounding gas. This allows for neglect of convective interactions within the spray, assuming that the drag force quickly equilibrates the differences between droplet velocities and the surrounding mean gas flow [35]. Consequently, the analysis can be simplified to a one-dimensional spherical symmetry form. This framework is based on the 1D multiphase droplet approach developed in [25], which demonstrated an accurate capture of evaporation and decomposition under SCR conditions. The present framework can be extended to account for drag effects via a Reynolds number based on the relative velocity ($u_d - u_f$), as empirical models show that these effects can be non-negligible [36].

Second, the characteristic time scale of the gas-phase flow is assumed to be much shorter than that of droplet evaporation and urea decomposition. As a result, the surrounding gas quickly relaxes to a quasi-steady state, allowing evaporation and decomposition to be treated independently of transient far-field flow variations. Under this assumption, droplets within a Lagrangian parcel experience effectively quiescent ambient conditions, consistent with the parcel modeling approach [37].

Third, a detailed model for the decomposition of urea in the liquid phase is considered and comprises 13 elementary reactions to accurately capture the reaction kinetics shown in Table S1 [38]. The interface between phases is well defined, with boundary conditions that incorporate the influence of liquid-phase reactions on product release.

Finally, the pressure is assumed to be constant and uniform throughout the domain, consistent with the slow-moving exhaust gas conditions, which are nearly incompressible. The liquid phase is treated as an ideal mixture within the relevant temperature range, where non-ideal effects can be neglected. These assumptions simplify the model while preserving the accuracy needed to describe the decomposition of urea under realistic SCR operating conditions.

2.2. 1D Spherical detailed droplet model

Under the assumptions described in Section 2.1, the evaporation and urea decomposition of an individual droplet are simulated using a detailed one-dimensional transient model [38]. The droplet is assumed to be spherical and isolated in an ambient environment at constant temperature.

The spherical symmetry of the droplet allows the 1D radial model to capture the spatial and temporal evolution of temperature, species concentrations, and reaction rates within the droplet. This approach resolves coupled heat transfer, mass diffusion, and chemical reactions while reducing computational cost, following the methodology of [25]. The results can be tabulated for efficient use in CFD simulations.

The model explicitly resolves the liquid-phase urea decomposition mechanism, which comprises 13 elementary reactions [10]. The key intermediate and product species tracked include urea, ammonia (NH_3), isocyanic acid (HNCO), cyanuric acid (cya), biuret (biu), triuret (triu) and ammelide (amd). These species fully characterize the thermal decomposition pathway of urea relevant for SCR applications.

2.3. Droplet interface state vector

The results of the detailed simulations are used to construct the state vector Ψ at the droplet interface for a given initial radius R_0 , ambient temperature T_0 , and time t . This state vector captures the effects of droplet evaporation and urea decomposition

$$\Psi(R_0, T_0, t) = (\dot{m}_{NH_3}, \dots, \omega_{urea(l)}, \dots, \dot{q}(t)), \quad (1)$$

where ω_i are the mass fractions of the condensed-phase species (solid and liquid), $\dot{m}_i$ are the mass fluxes of the gaseous species, and $\dot{q}$ is the energy flux at the droplet interface.

The tabulated interface data describe the instantaneous thermochemical state of the droplet. Consequently, all thermodynamic properties and species mass fractions are defined with respect to the current droplet mass at time t . The state vector therefore represents the evolving droplet composition during evaporation and decomposition.

All components of Ψ are obtained by solving the transient radial transport and reaction equations using the INSFLA in-house solver [25, 39]. These one-dimensional simulations provide accurate droplet-scale mass and energy fluxes, which can be directly used in CFD without resolving the detailed radial model.

2.4. Progress variable approach

To enable an efficient reduced description of the evolution of the UWS droplet, a scalar *progress variable* is introduced [25, 28]. The purpose of the progress variable is to map the complex, multi-physics transient behavior of a droplet for given boundary conditions – comprising evaporation, melting, chemical decomposition, and residue formation – onto a single monotonically increasing variable. This allows detailed 1D droplet solutions to be tabulated and efficiently accessed in CFD simulations without resolving the full internal droplet dynamics. The progress variable is constructed based on the observation that the evolution of a UWS droplet can be divided into four distinct and sequential stages, each

dominated by a specific physical or chemical process [25]. For each stage, a scalar quantity is selected that varies monotonically during that stage and remains approximately constant outside it. These quantities serve as local indicators of process development and are summarized in Table 1. In the present work, this progress-variable framework is employed to systematically investigate how variations in droplet-size distributions affect ammonia release and solid residual formation prior to wall impingement. In the first stage, water evaporation dominates the droplet behavior and is well described by the D^2 -law. Consequently, the normalized squared droplet diameter, $D^2 = (d/d_0)^2$, serves as a progress indicator. In the second stage, the melting of urea occurs at an approximately constant droplet diameter and is characterized by the liquid urea mass fraction, $\omega_{urea(l)}$. The third stage corresponds to the decomposition of urea and evaporation, during which the droplet temperature rises toward the ambient gas temperature; this process is captured by the normalized droplet temperature, T_d/T_g . Finally, the formation in the droplets of solid residues is represented by the triuret mass fraction, ω_{triu} , which increases monotonically during the last stage.

The progress variable φ is then defined as a weighted linear combination of each of the individual stage indicators:

$$\varphi = \alpha D^2 + \beta \omega_{urea(l)} + \gamma \frac{T_d}{T_g} + \delta \omega_{triu}, \quad (2)$$

where the weights α , β , γ , and δ are chosen so that φ increases monotonically throughout the lifetime of the droplet for the relevant ranges of droplet sizes and ambient temperatures. This ensures a unique mapping between φ and the droplet state for the considered ranges of the initial droplet radius and ambient temperature. Using φ as an independent coordinate, the results of the detailed 1D droplet simulations can be tabulated as functions of the progress variable. During coupled Euler/Lagrange CFD simulations, the local droplet state and the corresponding interfacial mass and energy fluxes are obtained by interpolation from this table, enabling

Table 1. Four stages of the UWS decomposition process and the corresponding progress-variable indicators

Stage	Description	Progress Variable (PV)
I.	Water evaporation with constant slope of D^2	D^2
II.	Urea is melted with approximately constant D^2	$\omega_{urea(l)}$
III.	Urea decomposition and evaporation with constant slope of D^2	T_d/T_g
IV.	Residual formation with approximately constant D^2	ω_{triu}

an accurate yet computationally efficient coupling between the reduced droplet model and the gas-phase flow solver. Details of the tabulation procedure and weight selection are provided in [28] and are briefly outlined in the next section.

The progress variable φ is defined as a linear combination of the stage indicators with weights α , β , γ , and δ , as given in Eq. (2).

2.5 Construction of the tabulated progress-variable Data

The parameter space considered in this study was chosen to cover application-relevant conditions for urea-water solution droplets. It comprises 20 initial droplet radii, ranging from 15 to 205 μm , and 36 ambient temperatures, ranging from 350 to 700 K, both uniformly distributed within their respective ranges (see Table S2). For all cases, the residence time is set to $t_{\text{res}} = 10$ s, ensuring complete droplet evaporation, urea decomposition, and solid residue formation under prescribed ambient conditions [40, 41]. The initial droplet composition is 32.5 wt% urea in 67.5 wt% water at 300 K, and the ambient gas corresponds to a typical diesel exhaust with 10 mol% H_2O , 10 mol% CO_2 , 10 mol% O_2 , and 70 mol% N_2 [40]. This setup results in a total of 720 detailed simulations, which are subsequently used to construct the tabulated progress-variable database for the reduced model.

Next, the weights α , β , γ and δ in the progress-variable definition (Eq. 2) are determined. For this purpose, the time derivative of the progress variable is approximated using finite differences between consecutive simulation points. Although the time steps are not strictly uniform, this approach provides sufficient accuracy for subsequent weight optimization and tabulation. The weights are then optimized by minimizing the variance of the derivative- $\dot{\varphi}$, ensuring a smooth and monotonic progression of progress variable. Finally, the progress variable φ is normalized to range from 0 to 1 (as defined in Eq. S1).

The entire decomposition process is tabulated as a function of the initial droplet radius R_0 , the ambient temperature T_0 and the progress variable φ with its derivative in time. Although the evolution of the droplet can be expressed through the dimensionless diameter D , using R_0 directly represents the initial condition, while φ captures the subsequent physical and chemical evolution. Thus, the state vector is defined as $\Psi(R_0, T_0, \varphi)$.

Following optimization, 100 uniformly spaced points along the progress variable are obtained by

interpolation. This discretization reproduces the results of the detailed 1D model with an accuracy within a few percent [28].

All tabulated quantities are indexed by the progress variable φ , which tracks the chemical and physical evolution of the droplet, including evaporation and decomposition of urea. Interpolation along φ is most accurate for droplets with similar initial radii and ambient temperatures, as their decomposition behavior is comparable. The resulting table represents droplet evaporation and urea decomposition as functions of the initial radius and ambient temperature, providing sufficient resolution throughout the ROI (see Table S3). This approach efficiently supplies CFD solvers with all required mass and energy exchange information without resolving the detailed 1D model.

2.6. Application of tabulated progress-variable Data

Once constructed, the tabulated data provide the system variables and the source terms associated with the progress variable, enabling direct integration into CFD simulations within a Lagrangian framework [28].

In the present study, the tables are employed as a stand-alone model to access droplet evaporation and urea decomposition properties. This allows systematic estimation and analysis of ammonia release and solid residue formation under conditions relevant to SCR applications. For individual droplet parcels in a stand-alone framework, the table provides evaporation rates and species mass fluxes at the droplet surface, which can be directly used as source terms in CFD solvers or reduced models. The heat flux per unit droplet surface area is also tabulated, allowing inclusion of the corresponding energy exchange as a sink in a CFD computational cell or in the stand-alone model.

The raw tabulated data (see Tables S4, S5 and S6), enable the direct retrieval of product masses. The masses of liquid and solid species are obtained from their respective mass fractions (properties see Table S3), while the masses of gaseous species are calculated by integrating the tabulated evaporation rates (properties 15–20) over time.

2.7. Reduced model

Building on the tabulated data described in the previous subsection, the reduced model provides a computationally efficient framework to evolve droplet properties in time without resolving the full 1D

detailed model. This approach allows for accurate prediction of droplet evaporation, urea decomposition, and species release within CFD simulations at low computational cost.

Accurate CFD predictions of droplet evaporation and urea decomposition rely on interpolated data sets that capture droplet behavior across the relevant ranges of initial radii and ambient temperatures. To achieve this, a detailed grid of precomputed droplet solutions was generated, covering the entire parameter space with sufficient resolution to reproduce the detailed 1D model within a few percent [28].

The evolution of the progress variable for each droplet parcel is computed recursively using a simple Euler integration,

$$\begin{cases} \varphi(t=0) = \varphi(R_0, T_0, 0), \\ \varphi(t+\Delta t) = \varphi(t) + \dot{\varphi}(R_0, T_0, \varphi(t))\Delta t, \end{cases} \quad (3)$$

where R_0 and T_0 denote the initial droplet radius and ambient temperature within the tabulated range, and t is the simulation time. First, the table is bi-linearly interpolated with respect to R_0 and T_0 to obtain system variables, including $\dot{\varphi}$. Then, the progress variable φ at time t is evaluated using the recursive Euler method (Eq. 3). Finally, the state vector of the droplet at t is obtained by interpolating the system variables along the calculated φ [28].

Thus, the state vector is approximated as

$$\Psi(R_0, T_0, \varphi(t))$$

providing an accurate yet computationally efficient description of droplet evolution for CFD simulations.

2.8. Spray modeling

To study the effect of the droplet-size distribution on evaporation and decomposition, several representative distributions are considered. Three discrete droplet size distributions are generated for all radii in the range of 15–205 μm (see Table S6), all sharing the same Sauter Mean Diameter (SMD = 117 μm , see Eq. S4), to isolate distribution effects while keeping the surface-to-volume ratio constant.

The mathematical definitions of these distributions are provided in the Appendix (Eqs. S2 and S3), along with appropriate references.

Three droplet-size distributions are considered, namely the Rosin–Rammler, double-hump, and double-hump2 distributions, whose parameters are summarized in Table 2. The Rosin–Rammler distribution serves as the reference case, while the double-hump distribution emphasizes a larger-droplet mode and the double-hump2 distribution represents a population dominated by smaller droplets. Figure 2 illustrates the corresponding frequency distributions as a function of the droplet radius approximated by the parcel approach.

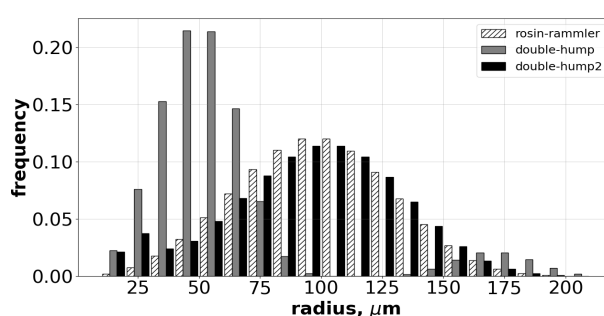


Fig. 2. Approximation by the parcel approach for droplet frequency versus radius for three distributions: Rosin–Rammler (single peak), double-hump (larger peak at small droplets), and double-hump2 (smaller peak at small droplets, larger peak aligned with Rosin–Rammler at large radii).

For a given droplet size distribution, spray quantities are obtained by superposition of the corresponding single-droplet results. Each discrete droplet radius R_i is associated with a probability p_i from the chosen distribution, with $\sum_{i=1}^N p_i = 1$. For any tabulated droplet property X (e.g. ammonia release, residue mass, or heat flux), the spray value is computed as

$$\sum_{i=1}^N p_i X(R_i, T_0), \quad (4)$$

where $X(R_i, T_0)$ is obtained from the reduced single-droplet table (see Sect. 2.6). This linear superposition assumes independent droplet behavior, neglecting inter-droplet interactions. Distribution effects are taken into account, while flow effects are neglected.

Table 2. Parameters of the considered droplet-size distributions (Eqs. S2 and S3)

Distribution	A [μm]	B [μm]	n	λ [μm]	λ_1 [μm]	λ_2 [μm]	α
Rosin–Rammler	15	205	3.5	110	–	–	–
Double-hump	15	205	3.5	55	–	–	0.0875
Double-hump2	15	205	3.5	–	25	110.3	0.05

3. Results and discussion

3.1. Preliminaries

This section presents the thermochemical evolution of UWS droplets using the reduced model and tabulated interface data. First, the reduced model is validated against detailed simulations and tabulated data. The droplet interface data are then examined to illustrate the temporal evolution of liquid, solid, and gaseous species. Finally, the effects of droplet radius, ambient temperature, and droplet-size distributions on ammonia and residue formation are analyzed.

Since all decomposition products except water originate from urea, normalized mass fractions are introduced to quantify decomposition and enable comparison across droplets of different initial sizes [28]. Two types are used:

Phase mass fractions relative to the initial droplet mass:

$$\omega_{\text{gas}}^0 = \frac{m_{\text{gas}}(t)}{m_d(0)}, \quad \omega_{\text{liquid/solid}}^0 = \frac{m_{\text{liquid/solid}}(t)}{m_d(0)}, \quad (5)$$

Here, $m_{\text{gas}}(t)$ is obtained by integrating the mass flux of evaporated species over time, and $m_{\text{liquid/solid}}(t)$ is the instantaneous mass of condensed components.

Species mass fractions normalized by the initial urea mass:

$$\omega_i^{u,0} = \frac{m_i(t)}{m_{\text{urea}}(0)}, \quad (6)$$

where $m_i(t)$ is the instantaneous mass of species i . This provides a consistent basis for comparing the formation of ammonia and residues across different droplet sizes.

These definitions provide a common framework for analyzing droplet composition and decomposition behavior under varying conditions.

3.2. Reduced model validation

To verify the reduced model, a droplet with an initial radius of 110 μm and ambient temperature 525 K, representing representative interior point of the tabulated parameter domain is considered. The results of the detailed simulations, tabulated data, bi-linearly interpolated table values, and the reduced model Euler integration of the interpolated data [28] are compared.

Figure 3 shows the mass fractions of liquid $\omega_{\text{urea}(l)}^0$ and ammonia $\omega_{\text{NH}_3}^0$. The reduced model reproduces the main trends of the detailed data, including peak timings and magnitudes, with minor quantitative deviations of few percent.

Liquid urea: The reduced model captures the increase during melting and subsequent decrease during decomposition (Fig. 3a). Relative errors in the maximum value are 0.03%, and deviations in peak time are 0.087 s.

Ammonia (gas-phase): The ammonia mass fraction $\omega_{\text{NH}_3}^0$ increases monotonically up to 10 s (Fig. 3b). Relative errors are 2.0% for the reduced model.

Overall, the reduced model reproduces the detailed simulations within a few percent. Minor discrepancies are attributed to interpolation and first-order time integration, confirming that the reduced model provides a reliable and computationally efficient surrogate across the tabulated parameter space.

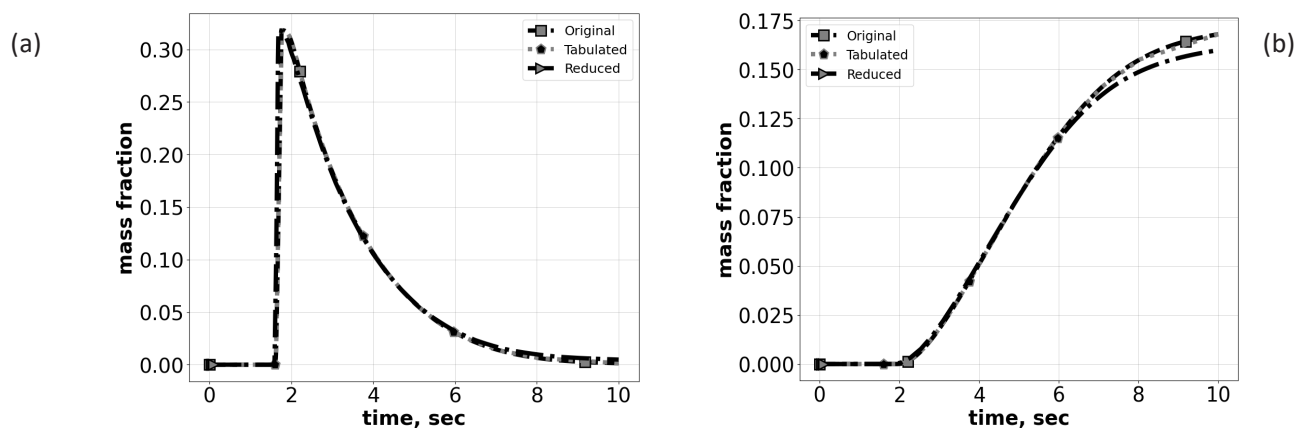


Fig. 3. Mass fraction of (a) liquid $\omega_{\text{urea}(l)}^0$ and (b) ammonia $\omega_{\text{NH}_3}^0$ for a 110 μm droplet at 525 K, comparing detailed simulations, tabulated data, and the reduced model.

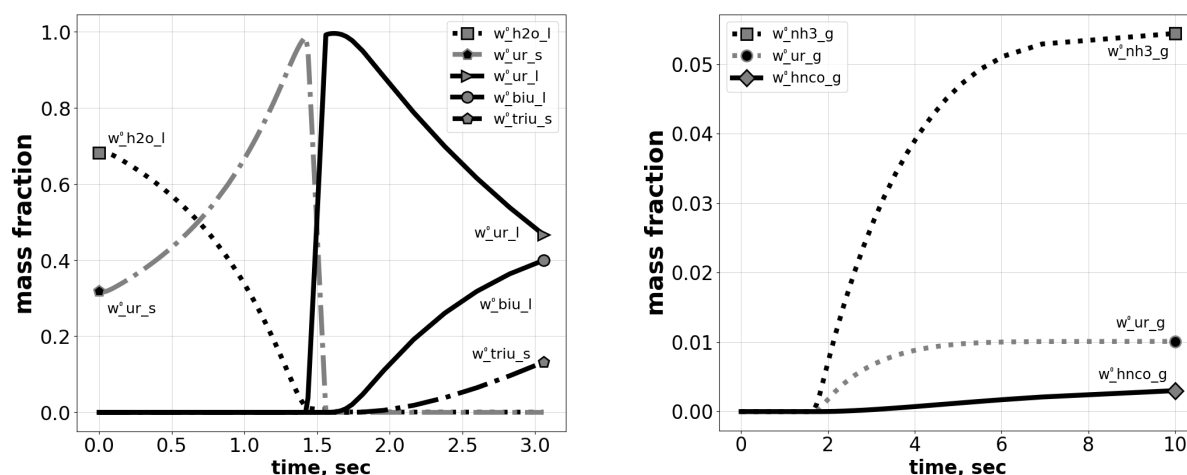


Fig. 4. Mass fractions of droplet components ω_i^0 (species symbol i listed in Table S2) for a droplet with an initial radius of 105 μm at 530 K. (a) Liquid and solid phases; (b) Gas phase (excluding water).

3.3. Interface data

The droplet interface provides detailed information on the decomposition process, including the formation of solid residues and the release of gaseous species.

Figure 4a shows the mass fractions of the main solid and liquid components ($\omega_{liquid/solid}^0$) during the first 3 s of decomposition. During the water evaporation stage (0–1.4 s), no chemical reactions occur. After evaporation, solid urea melts (1.4–1.6 s) into liquid urea, which subsequently decomposes. After 3 s, approximately 50% of the initial urea mass has decomposed. At 10 s, the liquid biuret becomes the dominant component, followed by the solid triuret residue, reaching roughly 40% and 13% of the droplet mass, respectively. All other liquid and solid residues remain negligible during this period.

The interface data also provide evaporation rates for each gaseous species. By integrating these rates over time, the gas-phase mass fraction can be obtained for each component. Figure 4b presents the evolution of all the major gaseous species except water ω_i^0 . NH_3 dominates the gas phase, reaching about 5.5% of the initial droplet mass. The urea vapor stabilizes at approximately 1% and isocyanic acid (HNCO) reaches approximately 0.2% at the end of the residence time.

In general, the interface data allow for full quantification of all droplet components, capturing both the formation and decomposition of solids and liquids, as well as the release of gaseous species such as NH_3 , urea, and HNCO.

3.4. The decomposition species dynamics

The tabulated data allow for tracking the evolution of all 15 species involved in the decomposition process. For clarity, non-water components are grouped into five categories: urea (solid, liquid, and gas), res(s) (solid residues), res(l) (liquid residues), res(g) (gaseous residues) and NH_3 (ammonia gas) (see Tables S2 and S3).

All decomposition products, except water, originate from urea. The mass fractions of all species are normalized by the initial urea mass (see Sect. 3.1), allowing for a direct comparison of the decomposition processes across droplets with different initial radii [28]. This convention ensures that ammonia and residue fractions are directly referenced to the urea that generated them.

Figure 5 illustrates the mass fractions of these groups at four characteristic stages for a droplet with an initial radius 105 μm at 530 K. Rows correspond to groups, and columns indicate individual species within each group. These fractions correspond to the species mass fractions $w^{u,0}$ introduced in Sect. 3.1, which are normalized by the initial urea mass.

Stage I (Fig. 5a, 1.08 s) corresponds to evaporation, with only solid urea present. Stage II (Fig. 5b, 1.49 s) marks urea melting. In Stage III (Fig. 5c, 2.38 s), liquid biuret dominates the residues, with some ammonia. Stage IV (Fig. 5d, 10.00 s) shows solid triuret as the main residue, with a notable fraction of ammonia.

Although the mass of ammonia is lower than that of triuret, its smaller molecular weight (17.03 vs. 146.11 g/mol) results in a comparable number of molecules (see Table S5).

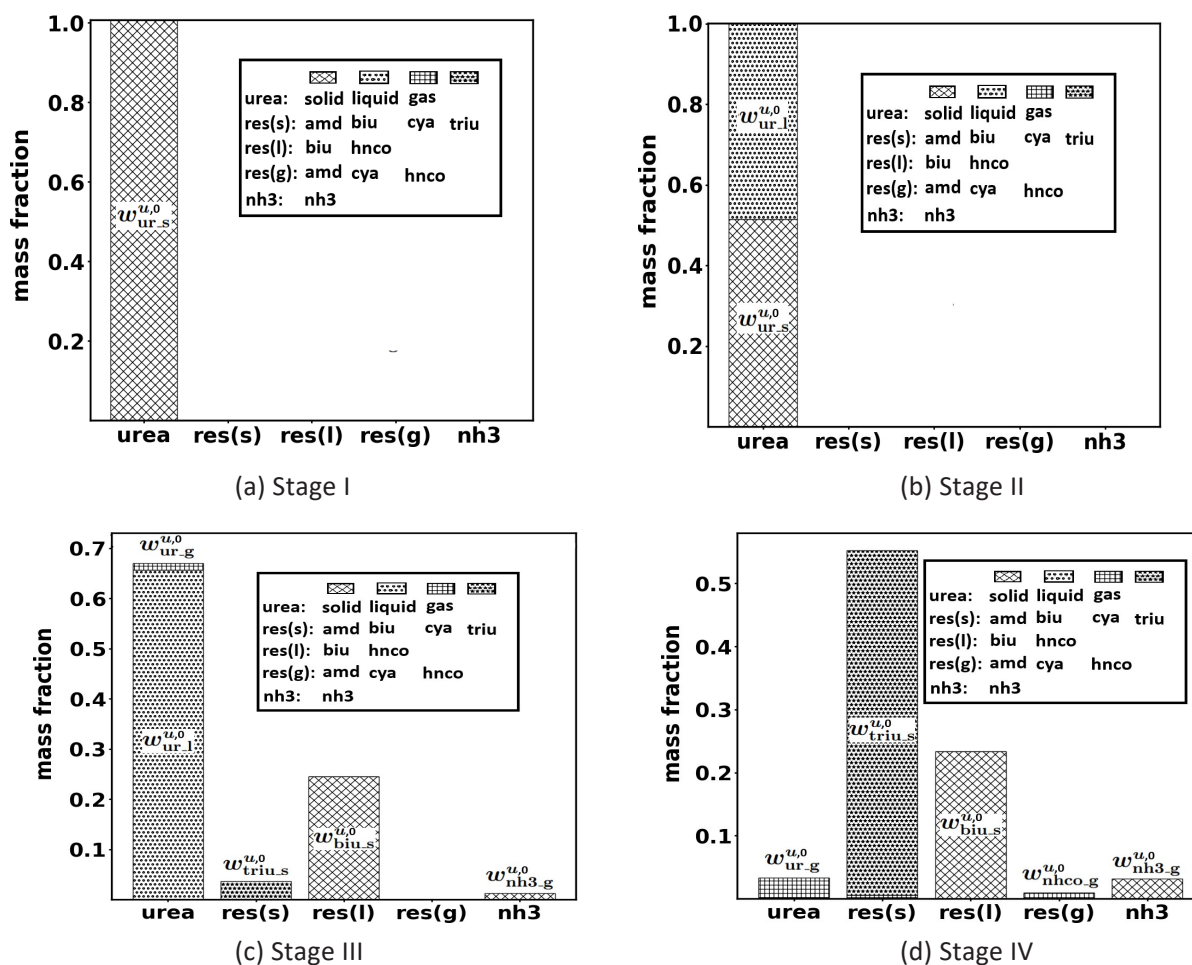


Fig. 5. Four stages of UWS decomposition for a droplet with initial radius 105 μm and ambient temperature 530 K. Each subfigure presents a matrix of species mass fractions $\omega_i^{u,0}$ (species symbol i listed in Table S2) normalized by the initial urea mass. Rows correspond to species groups (urea, res(s), res(l), res(g), nh3; listed in Table S2), while columns represent individual species within each group. (a) Stage I: evaporation; (b) Stage II: urea melting; (c) Stage III: liquid residues dominate; (d) Stage IV: solid residues dominate.

3.5. Effect of droplet radius and temperature on decomposition in a parcel

The influence of the initial droplet radius (fixed spacing) at 530 K and the ambient temperature (fixed spacing) at 105 μm on the mass fractions of triuret ($\omega_{triu}^{u,0}$) and ammonia ($\omega_{NH_3}^{u,0}$) is examined over a period of 10 s.

Figure 6a shows the triuret mass fraction, ($\omega_{triu}^{u,0}$), versus time for a fixed droplet radius of 105 μm at several ambient temperatures. Triuret formation occurs only for temperatures between 500 and 700 K. For high temperatures (600–700 K), the formation begins around 0.8–1 s. The maximum fractions at the end of the 10 s period are 18% (600 K), 14% (650 K) and 11% (700 K). At lower temperatures, formation starts later: 550 K at 1.8 s and 500 K at 2.7 s, reaching 18.5% and 8% at 10 s, respectively. For 650 K and 700 K, the triuret fraction decreases after 4 s

due to melting. In contrast, 550 K and 600 K stabilize near 18%, and 500 K continues to increase until the end of the simulation.

Figure 6b shows the triuret mass fraction, ($\omega_{triu}^{u,0}$), versus time for a fixed ambient temperature of 530 K and several initial droplet radii. All curves show an overall increasing trend. The onset of triuret formation occurs later for larger droplets, ranging from 0.1 s for the smallest droplets (15 μm) to 5.5 s for the largest droplet. Smaller droplets (15–95 μm) converge near 17.5 to 18.5% at 10 s, while larger droplets (125–225 μm) reach 3.7 to 17%, indicating a negative correlation between maximum triuret fraction and droplet size.

Figure 7a shows the ammonia mass fraction, ($\omega_{NH_3}^{u,0}$), versus time for a fixed droplet radius and several ambient temperatures. Noticeable production occurs only between 450 and 700 K, with 450 K reaching a maximum of 0.5% at the end of the

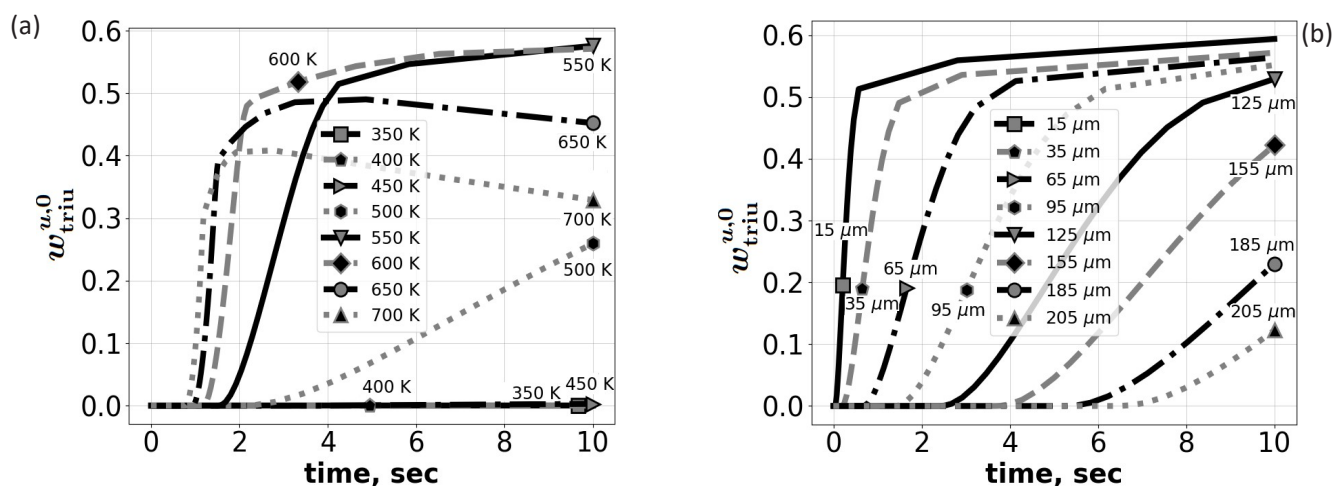


Fig. 6. Mass fraction of triuret ($w_{triu}^{u,0}$) versus time for two cases: (a) fixed initial droplet radius of 105 μm with varying ambient temperatures; (b) fixed ambient temperature of 530 K with varying initial droplet radii.

residence time. For 550–700 K, the onset times are similar to those of triuret formation, while 500 K and 450 K appear later, approximately 2 s and 3.5 s, respectively. The maximum ammonia fractions at the end of the residence time are 5.4% (550 K), 5.2% (600 K), 4.6% (650 K), 4.2% (500 K) and 4.0% (700 K). In general, the trend generally follows that of triuret formation, except that the values for 500 K become more dominant than those of 700 K at 9 s.

Figure 7b shows the ammonia mass fraction, ($w_{NH_3}^{u,0}$), versus time for a fixed temperature and several droplet radii. The trends are similar to those of triuret formation (Fig. 6b), with onset times that match the case of the triuret. At the end of the residence time, the smaller droplets (15–125 μm) converge around 5.35–5.45%, while the larger droplets (155, 185, 205 μm) show a negative correlation with size, reaching 5.0%, 3.8% and 2.8%, respectively.

Overall, the results show that both the ambient temperature and the initial droplet radius strongly influence the formation of triuret and ammonia. The production of ammonia and triuret is positively correlated and begins at similar times, reflecting the coupled nature of these reactions (see Table S4). Higher temperatures generally accelerate the onset of formation, with maximum triuret production occurring at intermediate temperatures (550–600 K) and decreasing at the highest temperatures due to melting. Ammonia exhibits a similar trend, with slight deviations at extreme temperatures.

The size of the droplet also plays a critical role: smaller droplets achieve higher triuret and ammonia fractions at the end of the residence time, while larger droplets show delayed onset and lower maximum production. The temporal profiles of triuret and ammonia are qualitatively similar, indicating that the trends for one species can inform predictions for

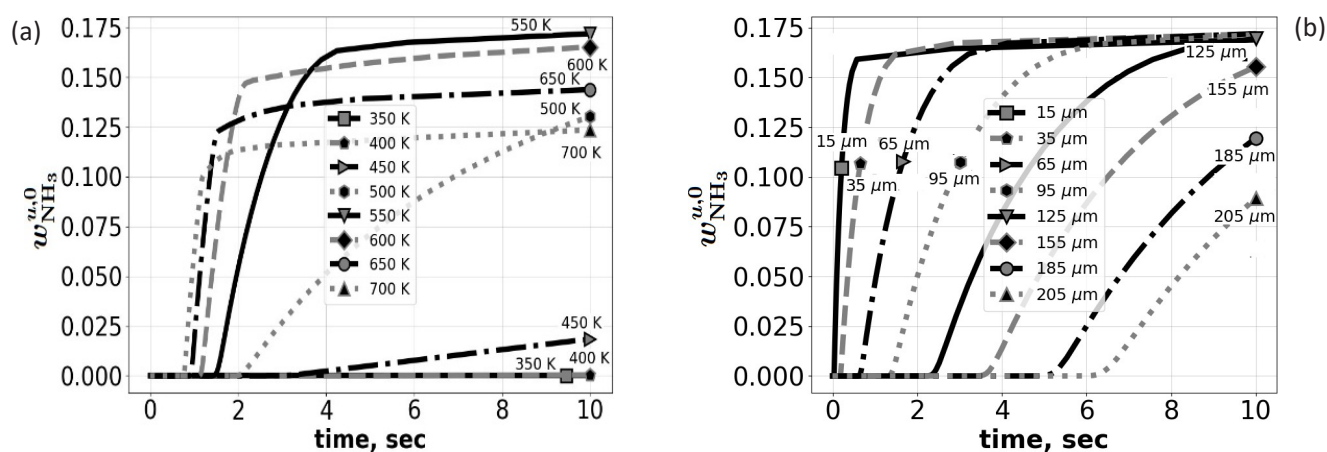


Fig. 7. Mass fraction of ammonia ($w_{NH_3}^{u,0}$) versus time for two cases: (a) a fixed initial radius of 105 μm for several ambient temperatures; (b) a fixed initial temperature of 530 K for several initial radii.

the other. This relationship links initial droplet conditions to the chemical composition present during wall-film formation, providing essential input for modeling downstream SCR processes and understanding the evolution of ammonia availability and solid residues.

3.6. Droplet-size distribution effects

To account for distribution effects and assess the validity of the SMD approximation, three different droplet size distributions with the same Sauter Mean Diameter (SMD) of 117 μm are considered: Rosin-Rammler, double-hump and double-hump2, as described in subsection 2.8.

Definitions. For each distribution, the mass fractions of ammonia and triuret are with respect to the initial urea in the residence time are denoted as

$$\omega_{\text{NH}_3,\text{end}}^{u,0} = \omega_{\text{NH}_3,\text{end}}^{u,0}(t = 10\text{s}), \quad \omega_{\text{triu},\text{end}}^{u,0} = \omega_{\text{triu},\text{end}}^{u,0}(t = 10\text{s}), \quad (7)$$

and the deviations relative to the SMD reference are defined as

$$\Delta\omega_{\text{NH}_3,\text{end}}^{u,0}(\text{dist}) = \omega_{\text{NH}_3,\text{end}}^{u,0}(\text{dist}) - \omega_{\text{NH}_3,\text{end}}^{u,0}(\text{SMD}), \quad (8)$$

$$\Delta\omega_{\text{triu},\text{end}}^{u,0}(\text{dist}) = \omega_{\text{triu},\text{end}}^{u,0}(\text{dist}) - \omega_{\text{triu},\text{end}}^{u,0}(\text{SMD}), \quad (9)$$

where $\omega_{\text{NH}_3,\text{end}}^{u,0}(\text{SMD})$ indicates the SMD reference case.

These definitions allow quantification of differences in chemical production due to the droplet-size distribution, independent of the specific temperature at which the maximum occurs. Figure 8a presents the ammonia mass fraction at the resonance time with respect to the initial urea as a function of temperature for the Rosin–Rammler, double-hump and double-hump2 distributions, together with the SMD approximation. For temperatures below ~ 520 K, the ammonia production is highest for the double-hump distribution, followed by the double-hump2, Rosin-Rammler and finally the SMD case. At higher temperatures ($T > 550$ K), this ordering reverses, with the SMD approximation yielding the largest ammonia production.

To quantify these differences, Fig. 8b shows the deviation in the ammonia mass fraction for each distribution relative to the SMD reference. Positive deviations occur primarily in the intermediate temperature range (450–530 K), reaching a maximum near 480 K. Negative deviations dominate at higher temperatures (550–700 K), with the largest differences observed near 700 K.

The mass fraction of triuret production in the resonance time with respect to the initial urea for the double-hump, double-hump2, Rosin-Rammler and SMD distributions versus temperature is shown in Fig. 9a. Figure 9b shows the deviation of the triuret production for the double-hump, double-hump2 and Rosin-Rammler distributions relative to the SMD reference versus temperature. Both graphs in Fig. 9 are positively correlated with the corresponding ammonia graphs in Fig. 8 and exhibit similar trends.

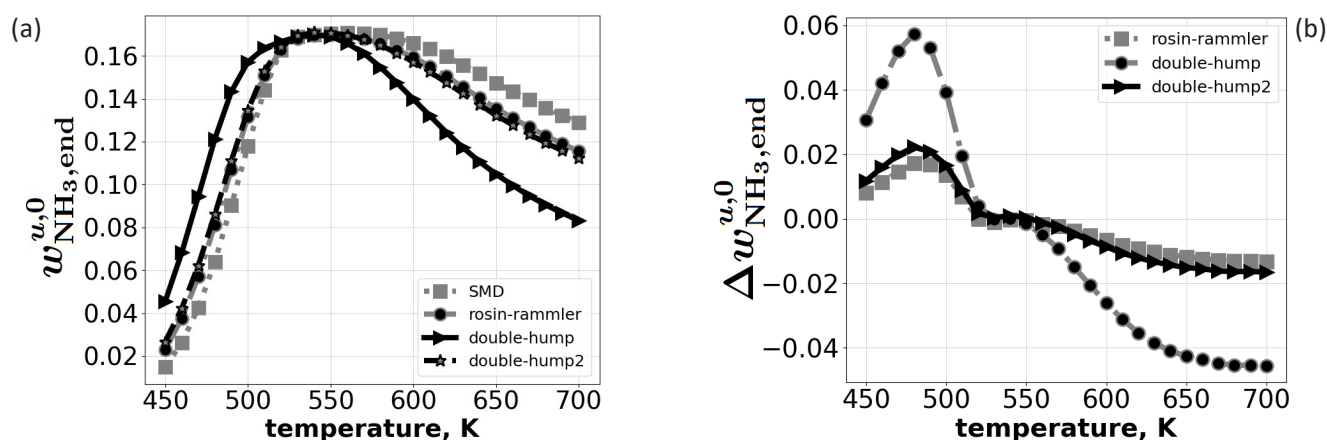


Fig. 8. (a) Mass fraction of ammonia at the residence time with respect to initial urea, $\omega_{\text{NH}_3,\text{end}}^{u,0}$ versus temperature for the double-hump, double-hump2, Rosin–Rammler, and SMD distributions. (b) Deviation of the ammonia mass fraction relative to the SMD reference, $\Delta\omega_{\text{NH}_3,\text{end}}^{u,0}$, for the double-hump, double-hump2, and Rosin–Rammler distributions.

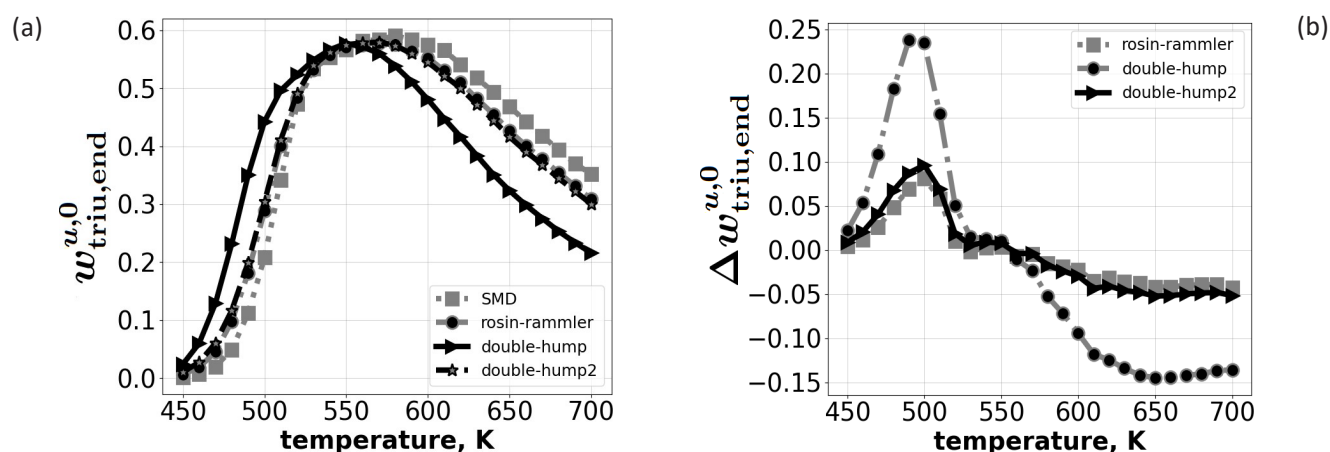


Fig. 9. (a) Mass fraction of triuret in the residence time with respect to initial urea, $\omega_{triu,end}^{u,0}$, versus temperature for the double-hump, double-hump2, Rosin-Rammler, and SMD distributions. (b) Deviation of the triuret mass fraction relative to the SMD reference, $\Delta\omega_{triu,end}^{u,0}$, for the double-hump, double-hump2, and Rosin-Rammler distributions.

Similarly to the previous section, the graphical profiles of ammonia and triuret show a positive correlation with high qualitative similarity, as seen in Figs. 9a and 8a, and likewise for the SMD difference plots in Figs. 9b and 8b. The Rosin-Rammler and double-hump2 distributions exhibit similar characteristics, since double-hump2 introduces a small fraction of smaller droplets compared to the Rosin-Rammler distribution. Specifically, the small droplets in the double-hump2 distribution are approximately one-quarter the radius of those in the Rosin-Rammler distribution, resulting in only a slight increase in the number of small droplets (5%), which translates to less than a 2% change in the overall volume of the droplets. Despite the similarity in the shapes of the general distribution, the differences in ammonia and triuret production between these two distributions exceed 20% in the 470–490 K range and at temperatures greater than 620 K, where production is highest, as reported in Table 3.

This amplified effect of a small fraction of fine droplets arises from the strong radius- and temperature-dependent behavior of urea decomposition. As shown in Figs. 6 and 7, small droplets contribute significantly to the formation of ammonia and triuret at low temperatures, whereas their contribution rapidly decreases at higher temperatures.

In contrast, droplets with radii close to the SMD, which dominate the spray volume, exhibit limited decomposition at low temperatures and rely on elevated temperatures for efficient product formation. Consequently, the small increase in fine droplets introduced by the double-hump2 distribution leads to improved production in the low-temperature regime (470–490 K), where medium droplets remain largely inactive. At higher temperatures ($T > 620$ K), the reduced contribution of fine droplets results in lower overall production compared to the Rosin-Rammler case. This temperature-dependent behavior explains why differences exceeding 20% arise despite a change of less than 2% in total droplet volume.

This analysis confirms that, although the Sauter Mean Diameter (SMD) provides a useful first-order characterization of the spray, subtle differences in the distribution of small droplets can significantly impact the chemical output, especially in temperature sensitive regimes. Fine droplets decompose more rapidly at lower temperatures, driving the early formation of ammonia and triuret, whereas droplets near the SMD dominate the overall volume and contribute mainly at higher temperatures. Therefore, accounting for the full droplet-size distribution, rather than solely relying on the SMD, is

Table 3. Absolute differences (%) in triuret (TRIU) and NH_3 production at representative temperatures between the Rosin-Rammler and double-hump2 distributions.

Temp (K)	470	480	490	500	510	520	600	610	620	630	640	650
TRIU (%)	37	28	21	16	16	44	24	19	25	23	22	20
NH_3 (%)	27	23	20	18	24	97	25	24	24	23	22	21

crucial to accurately predicting species formation across the temperature range encountered in practical applications.

Note that experimental investigations of UWS evaporation, spray behavior, and deposit formation have been reported in the literature [14, 15, 20, 24]. However, to the best of our knowledge, experimental studies specifically isolating the effect of droplet-size-distribution shape at fixed SMD are currently unavailable. Future experimental work targeting sprays with identical SMD but different distribution shapes would provide valuable validation of the trends identified in the present study. Moreover, the proposed reduced model provides a computational tool for assessing droplet-size-distribution effects and can support atomizer and spray design in SCR applications.

4. Conclusions

The UWS decomposition process relevant to the treatment of exhaust gasses was investigated. A reduced model for droplet evaporation and urea decomposition of UWS, constructed as a lookup table, was used to reproduce and quantify the effect of spray droplet distributions on urea decomposition. This approach allows for any practically required accuracy while enabling fast evaluations suitable for Lagrangian CFD implementation.

Analysis of droplet-size distributions shows that sprays with identical Sauter Mean Diameter (SMD) but differing distribution shapes, such as Rosin-Rammler, double-hump, and double-hump2 lead to significant differences in ammonia and triuret production. Even small variations, such as the slight addition of smaller droplets in the double-hump2 distribution, can change ammonia production by more than 20% in specific temperature ranges. These differences are most pronounced between 470–490 K and above 620 K, where the decomposition pathways are particularly sensitive to droplet size. Although these changes in the distribution shape may seem small, they have a considerable impact on the overall production of ammonia and triuret, demonstrating that SMD alone is insufficient to fully characterize UWS sprays. The small addition of smaller droplets to the double-hump2 distribution, for example, results in less than a 2% change in volume, but still leads to more than 20% differences in product formation. The proposed reduced model facilitates efficient CFD-based simulations of SCR systems, underscoring the importance of accurately accounting for even small variations in droplet-size

distributions. These variations can significantly affect ammonia release and solid residuals formation, thus improving the accuracy of the prediction of ammonia production and deposit formation in SCR applications. This leads to more efficient and accurate simulations of urea decomposition.

Overall, the results demonstrate that the droplet-size distribution during pre-impingement stage plays a decisive role in shaping ammonia release and solid residue formation, and consequently, in defining the conditions for subsequent SCR processes. Even for sprays with identical SMD, differences in distribution shape lead to substantial variations in ammonia availability and residual formation, determining the initial composition of the wall film and influencing decomposition processes within the film. These findings emphasize that resolving droplet-size distributions beyond the SMD is essential to accurately capture the coupled effects of NH_3 production and deposit formation in the overall SCR process. In addition, the reduced model provides an efficient computational tool for evaluating arbitrary droplet-size distributions and enables future optimization of spray characteristics under system level SCR objectives.

CRedit authorship contribution statement

Shlomo Hareli: Performed research, developed method, wrote paper. **Viatcheslav Bykov:** Designed research, developed method, reviewed and edited paper. **Ulrich Maas:** Designed research, developed method, reviewed and edited paper.

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.

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Supplementary material

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